



GEORGE E. BROWN, JR. SALINITY LABORATORY



### Biennial Report 1999-2000

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**Area Director** 

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#### INTRODUCTION

We exit one millennium and begin another with a new name and new challenges. On January 21, 2000, the U.S. Salinity Laboratory was renamed in honor of the late congressman George E. Brown Jr. who's legislative efforts to advance agricultural technology and international cooperation led to the construction and dedication of the new USDA-ARS Riverside facility. Our Laboratory has long been known for its cutting edge technology and joint science projects with other countries. Brown saw a need to improve the working conditions of agricultural scientists and fought for a decade to obtain funding to build a modern, state-of-the-art facility to replace the aging lab that had operated near Mount Rubidoux for 58 years. The new laboratory opened in 1995 and was renamed and dedicated to Congressman Brown after his death in 1999. The George E. Brown Jr. Salinity Laboratory continues to serve the research needs of U.S. agriculture through its relevant, productive and creative scientific research programs.

As water quality and quantity becomes limited globally, problems associated with salinity have increased dramatically. Since agriculture is by far the dominant user of most of our water supply, there is growing interest in increasing the efficiency of water management through reuse of agricultural drainage water and other water currently considered as municipal or industrial waste water. There is an increased demand for salinity assessment criteria and measurement methods and tools; and there is a greater need to make more reliable and useful decision support models available to growers, water and drainage districts, and state and federal decision makers. Public concern for environmental and human health and safety have resulted in demands to reduce the impact that agricultural practices have on loading groundwater and surface water with salts, pesticides, nitrates, and other potentially toxic ions. Human health and safety is an emergent research concern associated with water reuse. It will be up to our staff to address these important issues and to contribute, through research and technology transfer, to solutions.

Last year the Laboratory responded to the changing needs of the agriculture through the addition of a new research group. The Food Safety Research Group is focused on preventing contamination of surface and ground waters from microbiological and chemical contaminants from concentrated animal feeding operations. The new research project will be led by new hires Mark Ibekwe, Microbiologist and Scott Bradford, Soil Scientist. Pamela Watt, Microbiological technician was also hired to assist the group. Xuan Liu, Biological Science Technician also began work during the year and will be assisting Clyde Wilson in the Plant Science Unit. The Soil Physics and Pesticide Research Unit hired one postdoctoral scientist, Robert Dungan to study how soil microorganisms help degrade fumigants.

In 1999, Frank Dalton retired after over 20 years of Federal Service. Dr. Dalton has been a pioneer in developing a dynamic salinity stress index that characterizes the effects of variable soil and climate factors on plant response. This work is truly unique and creative and will lead to future understanding in plant salinity stress research.

Other retirements include Robert LeMert from the Soil & Water Chemistry group after 44 years of Federal Service and Gladys Greer, Administrative Officer, who retired from the Location Office after 58 years of Federal Service. Other significant highlights include National and Area Awards.

As usual, several Salinity Laboratory scientists were recognized for outstanding achievement during the year. Sabine Goldberg, Soil Scientist, received the Soil Science Society America Fellow Award in 1999 from USDA for her research on adsorption chemistry of nutrient and trace element anions in soils and the effect of variably-charged surfaces on soil structure. Dennis Corwin, Soil Scientist, received the Stanford University's Cox Professor Award in 1999 in recognition of the pioneering work and continued accomplishments for the application of Geographic Information Systems and other advanced information technologies to the assessment of non-point source pollutants in the vadose zone. Martinus Th. van Genuchten, Supervisory Soil Scientist/Research Leader, received the 1999 Don and Betty Kirkham Soil Physics Award for recognition of outstanding contributions in the area of soil physics. Many others received local awards for their excellent efforts in research, research support, and activities associated with outreach, safety and civil rights. Our research effort during the last two years, led by our 14 research scientists, yielded over 100 publications excluding abstracts.

In the coming years we look forward to new challenges, great scientific accomplishment, and continued improvement of our scientific effort and productivity.

Michael C. Shannon Director

#### GEORGE E. BROWN, JR. SALINITY LABORATORY STAFF

<u>NAME</u> <u>TITLE</u>

Alves, Bill Computer Specialist
Austin, Richard Electronics Technician

Bradford, Scott Soil Scientist

Carroll, Peggy Accounting Technician

Cliath, Mark Chemist

Collier, William Administrative Officer

Cook, Roberta Secretary (Physics & Pesticide)

Corwin, Dennis Soil Scientist
Dalton, Frank Soil Scientist
Donovan, Terry Agronomist

Draper, John Biological Technician (Soils)

Dungan, Robert Postdoc Scientist Ernst, Fred Soil Scientist

Fargerlund, JoAn Physical Science Technician

Faust, Steve Machinist

Forster, Harry Physical Science Technician

Gan, Jay Associate Researcher

Goldberg, Sabine Soil Scientist

Greer, Gladys Administrative Officer (retired 01/00)

Grieve, Catherine Plant Physiologist

Hopper, Jennifer Physical Science Technician Huber, Mike Engineering Technician

Ibekwe, M. Microbiologist

Jobes, Jack Agricultural Science Research Technician (Soils)

Layfield, Donald Analytical Chemist

Lebron, Inma Soil Scientist

LeMert, RoseAnn Physical Science Technician

LeMert, Robert Senior Farm Machinery Mechanic

Leij, FeikeSoil ScientistLeung, SuzannePostdoc ScientistLesch, ScottSenior StatisticianLiu, XuanPlant Physiologist

Luther, Sondra Secretary (Plant)
Manning, Bruce Soil Scientist

#### TITLE **NAME**

NAME	<u> IIILE</u>
Moore, JoAnn	Purchasing Agent
Mohanty, Binayak	Assistant Researcher
• • •	Statistician
Nash, Phyllis	
Orlauski, Janice	Office Assistant
Padgett, Karen	Secretary (Director)
Papiernik, Sharon	Soil Scientist
Rose Coons, JoAnne	Secretary (Chemistry)
Poss, Jim	Soil Scientist
Rhoades, James	Soil Scientist
Russell, Walt	Mathematician
Schaap, Marcel	Soil Physicist
Shannon, Mike	Director/Supvy. Research Geneticist
Shouse, Pete	Soil Scientist
Skaggs, Todd	Soil Scientist
Simunek, Jirka	Hydrologist
Suarez, Donald	Research Leader/Supvy. Geologist
Taylor, Chris	Chemist
van Genuchten, M. Th.	Research Leader/Supvy. Soil Scientist
Vaughan, Peter	Research Hydrologist
Vishteh, Nahid	Biological Science Technician
Wang, Dong	Soil Scientist
Watt, Pam	Microbiologist

Plant Physiologist Soil Scientist

Research Geneticist Staff Research Associate

Soil Scientist

Wilson, Clyde

Wood, Jim

Yates, Scott Zeng, Linghe

Zhang, Ping

#### 1999-2000 VISITING SCIENTISTS ON STAFF

(Argentina)

Maria Correa

(Belgium)

Fariborz Abbasi

Diederik Jacques

(China)

Weiiping Liu

Qi-Quan Wang

Chi-Chuang Wang

Shi-Kui Xue

Chengyi Zhao

Jianting Zhu

(Denmark)

Christen Borgesen

(Egypt)

Mohamed Elsayed Galal

Akmal Karimov

Ahmed H. Khater

Mohamed Eldayed Shahab Ahmed Ezzat Abdel Wahab

Basyouni Abdel Razak Zayed

(Hungary)

Attila Nemes

Tibor Toth

(India)

Lalit Arya

(Italy)

Paolo Castiglione

(Japan)

Takeshi Ishizaki

Qingli Ma

Naomasa Nishimura

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Appendix A

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# Laboratory Program

#### **HISTORY**

In May 1995, the George E. Brown Jr. Salinity Laboratory moved to a state-of-the-art facility on the campus of the University of California at Riverside. The laboratory, which was established in 1937, previously occupied 10 acres south of Mount Rubidoux in western Riverside.

The new building includes offices, constant temperature rooms, and 18 different laboratories. Four greenhouses and three environmental chambers are conveniently attached to the main building. A climate-controlled rhizotron, lysimeters and sand tank facilities are also located on USSL grounds, along with mechanical and electrical shops.

Sixteen permanent scientists as well as ten post-doctoral researchers and twenty technicians work under three research units: Soil-Water Chemistry and Assessment, Plant Science & Food Safety, and Soil Physics-Pesticides. Scientists from many foreign countries frequently visit the laboratory for education and technical exchange.

The laboratory works closely with USDA's National Resources Conservation Service (formerly the Soil Conservation Service) and the U.S. Bureau of Reclamation. Close cooperative relations are also maintained with the state agricultural centers around the world.

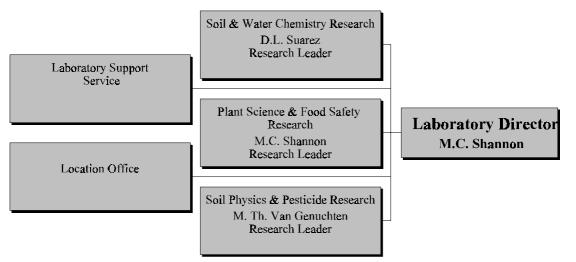
The George E. Brown Jr. Salinity Laboratory has served as a model for the establishment of Salinity Laboratories in India, Australia, Egypt, Israel, and Canada.

Irrigation is an ancient and yet important agricultural practice. Crop yields are higher under irrigation and less dependent on the effects of weather. While accounting for 0nly 15% of the world's cultivated land, irrigated soils produce 35-40% of the global food harvest; much more in semiarid and arid lands.

Unfortunately, irrigation often leads to the buildup of salts, toxic chemicals, and pesticides in associated soils and waters. Yield reductions related to salinity occur on an estimated 30% of irrigated land in the United States and 50% or more in some other nations. Approximately 10 million hectares (25 million acres) are permanently being lost each year from agriculture as a result of salinity and related problems.

The George E. Brown Jr. Salinity Laboratory is the nation's primary facility dedicated to basic research on salinity problems in agriculture. The laboratory is operated by the USDA Agricultural Research Service.

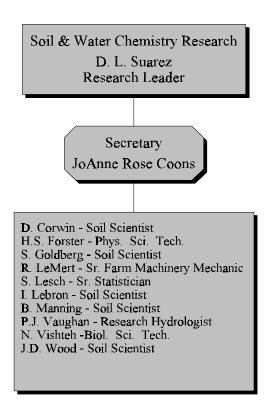
## **Laboratory Organization**



#### Mission

The George E. Brown Jr. Salinity Laboratory is a National Laboratory for basic research on the chemistry, physics, and biology of salt-affected soil-plant-water systems. The mission of its staff is to develop, through research, new knowledge and technology dedicated to the solution of problems of crop production on salt-affected lands, sustainability of irrigated agriculture, and degradation of surface- and ground-water resources by salts, toxic-elements, and pesticides.

# Soil & Water Chemistry Research



#### Mission

The mission of the Soil & Water Chemistry unit is to elucidate and quantify the chemical processes operative in salt-affected and/or sodic soils, including toxic elements; to develop instrumentation and technology for salinity measurement; and to develop control practices and agricultural management technologies to sustain irrigation while conserving soil and water resources. Major emphasis is to (1) develop models of the chemical and mineralogical controls of soil rootzones water compositions and (2) develop instrument-, tracer-, and GIS-techniques for the assessment and management of soil salinity and the determination of sources and magnitudes of salt loading. The specific objectives of the research program are to: (1) develop models and comprehensive criteria/standards to assess the suitability of salt-affected water for irrigation; (2) develop reclamation models; (3) develop knowledge necessary to predict mobility of potentially toxic trace anions, such as B, As, Se and Mo, in irrigated rootzones; (4) develop a methodology which uses geophysical measurements and image processing techniques to estimate the source and magnitude of salt discharges from irrigated soil; and (5) develop a GIS, and functional transport models to predict field-scale distributions of solute loading to groundwater.

#### SOIL & WATER CHEMISTRY RESEARCH STAFF



## DONALD L. SUAREZ, B.A., Ph.D., Research Leader and Supervisory Geologist of the Soil & Water Chemistry Research.

Water quality criteria for irrigation, predicting groundwater quality in relation to agricultural practices, modeling solute transport in soils, structural stability and reclamation of sodic soils and impact of irrigation on inorganic carbon budgets.

## SABINE GOLDBERG, B.S.A., Ph.D. Soil Scientist for Soil & Water Chemistry Research.

Trace elements adsorption reactions for predicting interactions with soil water in the irrigated root zone, chemical effects of salts on soil physical properties, structural stability of sodic soils.





# DENNIS L. CORWIN, B.S., Ph.D., Soil Scientist for Soil & Water Chemistry Research.

Development of management-oriented solute transport models to determine solute loading to the groundwater; measurement and assessment of soil salinity for the purpose of irrigation and drainage management; integration of solute transport models and geographic information systems for regional scale assessments and predictions of solute loading to the groundwater.

# JAMES D. RHOADES, B.S., M.S., Ph.D., Supervisory Soil Scientist for Soil & Water Chemistry Research.

Use of saline waters for irrigation; assessment of adequacy of leaching and drainage for salinity control; assessment of suitability of water for irrigation; soil salinity appraisal using geophysical instrumentation and use to assess the appropriateness of irrigation/drainage practices; and management to control pollution from irrigation/drainage.

# CHUNMING SU, B.S.C., M.S., Ph.D., Soil Scientist for Soil & Water Chemistry Research.

Partitioning of trace elements at interfaces between soil minerals and water; weathering of minerals in saline soils, and determination of B, Se and Mo speciation on oxide surfaces using FTIR.



### EVALUATION OF A SIMPLE LYSIMETER-DESIGN MODIFICATION TO MINIMIZE SIDEWALL FLOW

#### D.L. Corwin

A common criticism of many soil lysimeter designs has been the existence of artificial flowpaths along the soil-wall interface. This artificial flow is referred to as sidewall flow. A simple lysimeter-design modification was evaluated that utilizes annular rings to divert sidewall flow near the soil surface into the soil column to minimize the occurrence of sidewall flow along the remainder of the column's length. A chloride-tracer experiment was used to evaluate the effectiveness of annular rings in minimizing sidewall flow in a mesoscale soil lysimeter (0.6 m in diameter and 1.83 m in height). The tracer-experiment data showed that even though sidewall flow may not have been completely eliminated it was reduced to an undetectable level based on chloride distributions and time domain reflectometry measurements. However, a delicate balance exists between minimizing sidewall flow and significantly altering the natural water-flow dynamics when using annular rings. The simple design modification provides a means of using a disturbed column of soil to evaluate models of solute transport, and to study preferential flow and contaminant mobility without concern for spurious data due to artificial flow along the soil-wall interface of the lysimeter.

Journal of Contaminant Hydrology, 42:35-49, 1999.

### EVALUATION OF A GIS-LINKED MODEL OF SALT LOADING TO GROUNDWATER

#### D.L. Corwin, M.L.K. Carrillo, P.J. Vaughan, D.G. Cone and J.D. Rhoades

The ability to assess through prognostication the impact of nonpoint source (NPS) pollutant loads to groundwater, such as salt loading, is a key element in agriculture's sustainability by mitigating deleterious environmental impacts before they occur. The modeling of NPS pollutants in the vadose zone is well suited to the integration of a geographic information system (GIS) because of the spatial nature of NPS pollutants. The GIS-linked, functional model TETrans was evaluated for its ability to predict salt loading to groundwater in a 2396 ha study area of the Broadview Water District located on the westside of central California's San Joaquin Valley. Model input data were obtained from spatially-referenced measurements as opposed to previous NPS pollution modeling effort's reliance upon generalized information from existing spatial databases (e.g., soil surveys) and transfer functions. The simulated temporal and spatial changes in the loading of salts to drainage waters for the study period 1991-1996 were compared to measured data. A comparison of the predicted and measured cumulative salt loads in drainage waters for individual drainage sumps showed acceptable agreement for management applications. An evaluation of the results indicated the practicality and utility of applying a one-dimensional, GIS-linked model of solute transport in the vadose zone to predict and visually display salt loading over thousands of hectares. The display maps provide a visual tool for assessing the potential impact of salinity upon groundwater, thereby providing information to make management decisions for the purpose of minimizing environmental impacts without compromising future agricultural productivity.

J. Environ. Qual. 42(2):471-480, 1999.

### EVALUATION OF A FUNCTIONAL MODEL FOR SIMULATING BORON TRANSPORT IN SOIL

#### D.L. Corwin, S. Goldberg and A. David

There has been renewed interest in the application of functional models to the transport of nonpoint source pollutants at polypedon (i.e., farm) and watershed scales due to the ease of their coupling to a geographic information system and to the accepted organizational hierarchy of pedogenetic modeling approaches. However, very little work has been done to closely evaluate the performance of a functional transient-state model for the transport of a reactive solute over an extensive study period. The functional model TETrans was evaluated for model performance with boron (B) transport data collected from a soil lysimeter column over a 1000-day study period. Because the ability to simulate water flow has been previously evaluated for TETrans, the focus of this evaluation centered around the performance of various functional models of B adsorption used as subroutines within the TETrans model including the (1) Freundlich, (2) kinetic Freundlich, (3) Langmuir, (4) temperature-dependent Langmuir, and (5) pH-dependent Keren adsorption isotherm equations. Model performance was evaluated with statistical functions, and graphic displays of observed and predicted B concentration profiles. Results indicated that the order of model performance was the pH-dependent Keren equation first, followed by the kinetic Freundlich and Freundlich equations, the temperature-dependent Langmuir equation, and finally the Langmuir equation. Overall, the TETrans model was able to simulate the transport of B with deviations attributed to the fact that no functional adsorption equation incorporated all the influences of pH, ionic strength, temperature and kinetic effects into a single equation.

Soil Science 164(10):697-717, 1999.

# ADVANCED INFORMATION TECHNOLOGIES FOR ASSESSING NONPOINT SOURCE POLLUTION IN THE VADOSE ZONE: CONFERENCE OVERVIEW

## D.L. Corwin, K. Loague and T.R. Ellsworth

The information age has ushered in an awareness of and concern for global environmental problems such as climatic change, ozone depletion, deforestation, desertification, and nonpoint source (NPS) pollution. Nonpoint source pollution is the single greatest threat to surface and subsurface drinking water resources. Nonpoint source pollutants also pose a threat to sustainable agriculture, which is viewed as the most viable means of meeting the food demands of a world population that is expected to reach 9.4 billion by the middle of the next century. The ability to accurately assess present and future NPS pollution impacts on ecosystems ranging from local to global scales would provide a powerful tool for environmental stewardship and guiding future human activities. Assessing NPS pollutant is a multidisciplinary problem. To address the problem, advance information technologies and methodologies are needed that draw from all areas of science and are applied in a spatial context. It was from this setting that the 1997 Joint AGU Chapman/SSSA Outreach Conference Application of GIS, Remote Sensing, Geostatistics, and Solute Transport Modeling for Assessing Nonpoint Source Pollutants in the Vadose Zone (19-24 October 1997, Riverside, CA) materialized. The objective of the conference was to examine current multidisciplinary technologies and methodologies for assessing NPS pollutants in the vadose zone, and to explore new conceptual approaches. It was the conference's goal to provide a forum to stimulate multidisciplinary interactions to enhance the development of techniques for the realtime measurement and modeling of NPS pollution in the vadose zone and subsurface waters.

J. Environ. Qual. 28(2):357-365, 1999.

# REGIONAL SCALE ASSESSMENT OF NON-POINT SOURCE GROUNDWATER CONTAMINATION

### K. Loague and D.L. Corwin

Predictive assessments of non-point source (NPS) pollution can have great utility for environmentally focused land use decisions related to both the remediation of existing groundwater contamination and the regulation of current (and future) agrochemical use. At the regional scales associated with NPS agrochemical applications there are staggering data management problems in assessing potential groundwater vulnerability. Geographical information system (GIS) technology is a timely tool that greatly facilitates the organized characterization of regional-scale variability. In this paper we review the recently reported (Loague et al., 1988a,b) simulations of NPS groundwater vulnerability, resulting from historical applications of the agrochemical DBCP (1,2-dibromo-3chloropropane), for east-central Fresno County (California). The Fresno case study helps to illustrate the data requirements associated with process-based three dimensional simulations of coupled fluid flow and solute transport in the unsaturated/saturated subsurface at a regional scale. The strengths and weaknesses of using GIS in regional-scale vulnerability assessments, such as the Fresno case study, and the critical problem of estimating the uncertainties in these assessments (owing to both data and model errors) are discussed. A regional GIS-driven integrated assessment approach is proposed, which is based upon cost-benefit analysis, and incorporates both physical and economic factors that can be used in a regulatory decision process.

In: A.M. Gurnell and D.R. Montgomery (eds). "Hydrological Applications of GIS", John Wiley & Sons, Chapter 10 p.137-145, 2000.

# INVERSION OF SOIL CONDUCTIVITY PROFILES FROM ELECTROMAGNETIC INDUCTION MEASUREMENTS: 2. EXPERIMENTAL VERIFICATION

# J.M.H. Hendrickx, J.D. Rhoades, D.L. Corwin, S.M. Lesch, A.C. Hilgendorf and B. Borchers

Non-invasive electromagnetic (EM) induction techniques are increasingly being used for salinity monitoring of agricultural lands and contaminant detection in soils and shallow aquifers. The physical relationships between the apparent electrical conductivity (EC<sub>a</sub>) of a homogeneous semi-infinite half space and the response of an EM ground conductivity meter are well understood. Although theoretical considerations indicate the validity of these depth response functions or forward models for heterogeneous profiles, no experimental data have been presented to verify this assumption. The objectives of this study are twofold. The first one is to experimentally verify whether the linear and non-linear electromagnetic forward models for homogeneous media are valid in heterogeneous soil profiles. The second objective is the experimental verification of linear and non-linear methods for inversion of soil conductivity profiles using above-ground electromagnetic induction measurements with the EM38 ground conductivity meter. Experimental data from fourteen representative saline soil profiles in California have been used for the verification of linear and non-linear forward and inverse models. The linear and non-linear forward models derived for homogeneous media are indeed valid in heterogeneous soil profiles. However, since the errors of the linear forward model are approximately double those of the nonlinear forward model, the latter is the preferred one. No such difference was found between the linear and non-linear inverse models. In this study the linear inverse model outperforms the nonlinear model at EM38 measurements below 150 mS/m while at higher conductivities the non-linear inverse model yields slightly better results. The linear model is preferred since it needs considerably less computer resources.

Soil Sci. Soc. Am. J., (accepted) 2000.

# SOLUTE CONTENT - SUCTION CUPS, POROUS MATRIX SENSORS, ELECTRICAL RESISTIVITY

### J. M. Hendrickx, D.L. Corwin, J. Wraith and R.G. Kachanoski

Soil consists of solid, liquid, and gas phases. The measurement of the solute content of the soil solution is a quantification of the chemicals that are present in the liquid portion of the soil. This provides a means of determining the level of contamination and degradation status of the soil. The liquid phase of the soil is significant because it allows contaminants to move through the soil via diffusion or mass transport. A discussion of the principles, equipment, procedure and comments regarding the measurement of solutes in the soil solution with suctions cups, porous matrix sensors and electrical resistivity is presented. The discussion is part of the Solute Content Chapter of the Soil Science Society of America's Agronomy Monograph No. 9 Methods of Soil Analysis 3rd Edition. The discussion is designed to provide researchers with the background, latest equipment, and current accepted procedures and methodology for measuring solute concentration in the soil solution (particularly of soil salinity) with suction cup extractors, porous matrix/salinity sensors, and electrical resistivity.

SSSA Agronomy Monograph #9, Methods of Soil Analysis (3rd Edition) Chapter 6.1. 2000.

# SIMULATING MOLYBDENUM TRANSPORT THROUGH THE ROOT ZONE IN A SOIL LYSIMETER

## D.L. Corwin, S. Goldberg and A. David

Due to the ease of their coupling to a geographic information system and to the accepted organizational hierarchy of pedogenic modeling approaches, there has been renewed interest in the application of functional models to the transport of non-point source pollutants. A functional model of solute transport was used to simulate molybdenum movement through a mesoscale soil lysimeter column (0.6 m diameter, 1.83 m length) over a 1000-day study period. The focus was upon a comparison of the performance of various functional models of molybdenum adsorption used within the transport model including the (1) Freundlich, (2) kinetic Freundlich, (3) Langmuir, (4) temperature-dependent Langmuir, and (5) ph-dependent adsorption isotherm equations. Measured and simulated distributions of soil solution molybdenum were compared at depths of 0.15, 0.45, 0.75, 1.05 and 1.35 m. The model was best able to simulate the transport of molybdenum at the intermediate depths of 0.45 and 0.75 m and to a lesser extent the deeper depths of 1.05 and 1.35m, but was unable to reliably predict the shallowest depth. Failure to predict the shallowest depth was attributed to the methodology, specifically the inability to consistently collect soil solution extracts at field capacity.

Agronomy Abstract p. 345, 1999.

## DETECTION OF SOIL SALINITY EFFECTS ON SUGAR BEETS USING MULTISPECTRAL REMOTE SENSING

G.J. Fitzgerald, S.R. Kaffka, D.L. Corwin, S.M. Lesch and S.J. Maas

High resolution multi spectral remotely sensed imagery was acquired on four dates during the 1999 growing season for sugar beet field near Stratford, California using the Shafter Airborne Multispectral Remote Sensing System (SAMRSS), a digital airborne imaging system developed by the USDA-ARS laboratory at Shafter, CA. It consists of three digital cameras fit with specially coated filters allowing narrow band transmission of light at 550nm (green), 660 nm (red), and near infrared (850nm) wavelengths. Ground soil salinity was measured based on soil electrical resistivity measurements taken at over 3100 locations in the 160 acre study area. A soil salinity map of the field was generated using the resistivity measurements and associated soil core samples taken at 1 foot increments down to 4 feet at 19 statistically selected locations. Yield data were collected in small plots for root quality determinations and with a yield monitor mounted on a sugar beet harvester to estimate root yield. These data were correlated to the images collected to determine relationships between the images, soil salinity, and yield.

Agronomy Abstract p. 17, 1999.

### SOIL EC THEORY AND PRINCIPLES: WHAT IS IT AND HOW DOES IT WORK?

### D.L. Corwin

A general overview of the measurement of soil salinity using various electrical conductivity (EC) measurement techniques (i.e., soil-matrix salt sensors; electrical resistivity methods such as four-electrode probe and Wenner array; and electromagnetic induction) is presented with particular emphasis on spatial EC measurements. The following areas are discussed in the overview: brief history of the measurement of soil salinity, basic theories and principles of soil electrical conductivity measurement, electrical conductivity measurement techniques, examples of spatial EC measurement studies, applications and value of spatial measurements of soil EC to precision agriculture, and current/future developments.

Agronomy Abstract p. 77, 2000.

# FIELD SCALE ELECTRICAL CONDUCTIVITY AND CROP PRODUCTION IN CALIFORNIA

S.R. Kaffka, D.L. Corwin and S.M. Lesch

There has been little assessment of yield variation at the field scale in California. Two salt-affected fields, one in the Imperial Valley (IV) and one in the San Joaquin Valley (SJV), were assessed under uniform moisture conditions using electromagnetic induction (EM) methods and planted to sugarbeets. Both field scale yield maps and hand samples from sites identified based on survey data using a multiple regression algorithm were derived. Electrical conductivity (ECe) varied from 2 to 9 dS m-1 at the IV site, and from 3 to 24 dS m-1 at the SJV site. Percent seedling establishment declined from approximately 70% to 40% over the ECe range observed. Sugar yields varied within the field from 13.4 to 17.7 Mg ha-1, but was not significantly correlated with ECe. Sucrose concentration in roots increased significantly from 16.4 to 19.3 mg kg-1 in response to increasing ECe. At the SJV site, root and sucrose yield (2.9 to 14.2 Mg ha-1) responded more to soil texture, represented by soil saturation percentage (SP), but was positively correlated with ECe. Sucrose concentration varied from 15.0 to 18.7 mg kg-1, but was not affected by ECe. Different sugarbeet responses to ECe at the two sites are related to irrigation methods and more difficult management conditions at the SJV site.

Agronomy Abstract p. 80, 2000.

# THE INFLUENCE OF SALINITY ON SPATIAL VARIABILITY OF 13C NATURAL ABUNDANCE IN PLANT AND SOIL

## J.W. Van Groenigen, D.L. Corwin, W.R. Horwath and C. Van Kessel

Salinity-induced stress will cause plants to partially close their stomata. This will lead to a relative enrichment with 13C, and corresponding higher [delta]13C values in organic matter. The objective of this study was to explore the possibility of using differences in [delta]13C values in plant and soil organic (SOM) fractions to reconstruct the salinity history of a field. We compared spatial patterns of salinity, [delta]13C of the SOM and [delta]13C of corps on a Lethent Clay Loam in San Joaquin Valley, California. The ECa values ranged from 3 to 18 dS m-1 and [delta]13C values of the crop and SOM ranged from -29.8 to -24.0% and -25.3 to -21.4%, respectively. Spatial patterns of salinity and [delta]13C crop was highly correlated, with higher [delta] values associated with higher salinity. There was no relation between salinity and [delta]13C SOM patterns. Therefore we concluded that current salinity is likely of recent origin. To verify this conclusion, the [delta]13C patter of the light SOM fraction, which is considered to be the youngest SOM pool, should reflect the spatial salinity pattern. By distinguishing between [delta]13C values of the light

SOM fraction and older physical or chemical SOM fractions, the historic pattern of salinity stress can be reconstructed.

Agronomy Abstract p. 309, 2000.

# FIELD-SCALE SOIL ELECTRICAL CONDUCTIVITY CHARACTERISTICS AND SUGARBEET EMERGENCE, GROWTH, AND YIELD

S. R. Kaffka, D. L. Corwin, S. M. Lesch and G. Fitzgerald

An assessment of field-scale variation and the characterization of correlated crop response to this variation are first steps in evaluating the potential for variable rate technologies and other aspects of precision agriculture. As an initial attempt at site characterization, the response of sugarbeets to salinity and residual nitrogen was studied at sites in the Imperial and San Joaquin Valleys. Evaluation of the usefulness of salinity assessment technology developed by Rhoades and fellow workers at the U.S. Salinity Laboratory for precision agricultural management and the possible correlation of salinity and nitrate, especially deeper in the soil profile, were the objectives of this study. Nitrate was found to correlate with  $EC_e$  and  $EC_a$  (electrical conductivity of the saturation paste and bulk soil, respectively) at depth. This means that higher  $EC_a$  values can be used as a means of identifying likely locations in the profile to sample for residual  $NO_3$ -N. For sugarbeets, nitrate deep in the soil profile can lead to reduced sugar concentrations in the roots. The use of soil electrical conductance to evaluate variation in soil residual nitrate may make field scale assessment for this purpose far less expensive and much more practical and accurate than other ground-based attempts reported previously, and allow for sufficient amounts of data to be collected to make precision agricultural practices profitable.

Proceedings California Plant & Soil Conference, Stockton, CA, Abstr. p. 17, 2000.

# REANALYSIS OF BORON ADSORPTION ON SOILS AND SOIL MINERALS USING THE CONSTANT CAPACITANCE MODEL

## S. Goldberg

The constant capacitance model is shown to provide a quantitative description of boron adsorption on various aluminum and iron oxides, clay minerals, and arid zone soils as a function of solution pH. In the present model application, both trigonal and tetrahedral boron surface complexes are postulated, consistent with experimental spectroscopic results. Average sets of boron surface complexation constants for aluminum and iron oxides and kaolinites are not statistically significantly different from each other. Average sets of boron surface complexation constants for kaolinites are statistically significantly different from those for 2:1 clays and soils. Average sets of boron surface complexation constants for 2:1 clays and soils are not statistically significantly different from each other reflecting the dominance of 2:1 clay minerals in boron adsorption reactions in these arid zone soils. Average sets of boron surface complexation constants provided adequate descriptions of boron adsorption behavior on all adsorbents studied, indicating some predictive capability. The constant capacitance model was able to predict boron adsorption behavior on additional arid zone soils using the average set of boron surface complexation constants.

Soil Sci. Soc. Am. J. 63(4):823-829, 1999.

### SOIL COLLOIDAL BEHAVIOR

## S. Goldberg, I. Lebron and D.L. Suarez

Recent understanding that organic and inorganic contaminants are often transported via colloidal particles has increased interest in colloid science. The primary importance of colloids in soil science stems from their surface reactivity and charge characteristics. Characterizations of size, shape, surface area, and surface charge density are required for understanding the processes of adsorption, flocculation, dispersion, and transport in soils and the resultant changes in soil hydraulic properties as well as chemical migration. Colloids are reactive not only because of their total surface area but because of enhanced reactivity related to rough surfaces and highly energetic sites, as well as the effects of electrostatic charge. Colloid charge is associated with substitution of lower charge cations for those of higher charge in the mineral lattice as well as surface charge associated with broken bonds. The charge associated with broken bonds is characterized as variable charge in as much as the solution influences the surface speciation. In addition to these chemical processes, colloids are mobile in soils and thus affect not only the chemical transport of otherwise immobile chemicals but also exert a strong influence on soil hydraulic properties. Prediction of transport of pathogens (viruses and bacteria), radionuclides, heavy metals and organic contaminants require consideration of colloid mobility and thus understanding of both physical processes as well as surface chemistry. We review the general principles pertaining to these processes.

In: Malcolm E. Sumner (ed.) "Handbook of Soil Science", Section II, Soil Chemistry, Chapter 6, p. B195-B240, CRC Press, Boca Raton, FL, 1999.

# PREDICTING BORON ADSORPTION BY SOILS USING SOIL CHEMICAL PARAMETERS IN THE CONSTANT CAPACITANCE MODEL

## S. Goldberg, S.M. Lesch and D.L. Suarez

The constant capacitance model, a chemical surface complexation model, was applied to B adsorption on 17 soils selected for variation in soil properties. A general regression model was developed for predicting soil B surface complexation constants from easily measured soil chemical characteristics. These chemical properties were cation-exchange capacity (CEC), surface area, organic carbon content (OC), and inorganic carbon content (IOC). The prediction equations were used to obtain values for B surface complexation constants for 15 additional soils, thereby providing a completely independent evaluation of the ability of the constant capacitance model to fit B adsorption. The model was well able to predict B adsorption on the 15 soils. Incorporation of these prediction equations into chemical speciation-transport models will allow simulation of soil solution B concentrations under diverse environmental and agricultural conditions without the requirement of soil specific adsorption data and subsequent parameter optimization.

Soil Sci. Soc. Am. J. 64:1356-1363, 2000.

# PREDICTION OF BORON ADSORPTION IN SOILS USING THE CONSTANT CAPACITANCE MODEL

## S. Goldberg, S.M. Lesch and D.L. Suarez

The constant capacitance model, a chemical surface complexation model, was applied to boron adsorption on 14 assorted arid-zone soil samples. In agreement with previous spectroscopic results, we specified both trigonal and tetrahedral surface configurations for adsorbed boron. A general regression model was developed for predicting soil boron surface complexation constants from easily measured chemical soil characteristics. These chemical properties were cation exchange capacity, surface area, organic carbon content, and inorganic carbon content. The prediction equations were used to obtain values of boron surface complexation constants for four independent soils. Since the data from the four soils had not been used to develop the prediction equations, this is a completely independent evaluation of the ability of the general regression model to predict boron adsorption. The model was well able to predict boron adsorption on additional arid-zone soils from the Central Valley of California. The data base has been expanded and the regression model will be refined by including 16 additional soils having broader ranges of chemical characteristics.

ENVR 118, 217th ACS National Meeting, Anaheim, CA, Abstr., 1999.

# COMPETITIVE ADSORPTION OF ARSENATE AND ARSENITE SPECIES ON OXIDES AND CLAY MINERALS

## S. Goldberg

Arsenic is a toxic trace element for animals including humans. EPA proposes to significantly lower the As drinking water standard within the next year. Adsorption reactions on soil mineral surfaces potentially attenuate toxic soil solution As concentrations reducing contamination of groundwaters. Arsenic adsorption on amorphous aluminum and iron oxides and the clay minerals, kaolinite, montmorillonite, and illite was investigated as a function of solution pH and arsenic redox state. Arsenic adsorption experiments were carried out in batch systems to determine adsorption envelopes, amount of As(III) and/or As(V) adsorbed as a function of solution pH per fixed total As concentration. The constant capacitance model was able to fit the arsenate and arsenite adsorption envelopes to obtain values of the intrinsic As surface complexation constants. These intrinsic surface complexation constants were then used in the constant capacitance model to predict competitive arsenate-arsenite adsorption from solutions containing equimolar As(III) and As(V). The constant capacitance model was well able to predict As adsorption from mixed As(III)/As(V) solutions.

Agronomy Abstract p. 223, 2000.

## SATURATED HYDRAULIC CONDUCTIVITY AS AFFECTED BY PORE SIZE AND PORE GEOMETRY IN SOILS WITH VARIABLE CHEMICAL COMPOSITION

## I. Lebron, M.G. Schaap and D.L. Suarez

The methodology presented in this work consists in the analysis of binary images collected with a back scattered electron detector from thin sections of soils. Maximum and average diameter, surface area, perimeter, roughness and circularity were quantified. Saturated hydraulic conductivity ( $K_{sat}$ ) was measured in 36 undisturbed soils, particle size distribution, particle density, bulk density and chemical properties were determined in half of the core, the other half was used to prepare thin sections. We used the Kozeny-Carman equation to predict  $K_{sat}$  from the microscopic measurements, and neural network analysis to predict the formation factor from microscopic, macroscopic, and chemical data. Formation factor was best predicted when % clay, bulk density, roughness, and pH were used in the neural network and bootstrap approach. The predicted  $K_{sat}$  was in excellent agreement with the measured  $K_{sa}(R^2=0.97)$  when a hydraulic radius defined as  $r_H=area/perimeter$  was used. Area and perimeter are direct measurements obtained from the back scattered images. The improvement in our  $K_{sat}$  predictions when  $r_H$  is used instead of an average radius indicates that

the methodology proposed in this study may be useful to improve our capability to predict hydraulic properties.

Water Resources Research 35(10):3149-3158, 1999.

# MODELING CALCITE PRECIPITATION AS AFFECTED BY P<sub>CO<sub>2</sub></sub> AND ORGANIC LIGANDS AT 25°C

### I. Lebron and D.L. Suarez

We found that the DOC affects both crystal growth and heterogeneous nucleation at the three  $P_{CO_2}$  values studied. The precipitation rate of calcite in the range of  $\omega = 2.5-20$  decreased when the  $DO\bar{C}$  concentration increased for  $P_{CO_2}$  0.035, 5, and 10 kPa, however higher DOC concentrations were needed to cause an equal reduction in the precipitation when the P<sub>CO</sub>, increased. Calcite precipitation studies are generally performed in clean systems ad measure the effects of pH and  $P_{CO_2}$ on calcite precipitation at different temperatures for crystal growth. However, water soluble organic ligands and ions such as PO<sub>4</sub><sup>3</sup>-have been known to act as precipitation inhibitors by blocking crystal growth sites. In a seeded crystal growth experiment Inskeep and Bloom (1986) found that the precipitation rate constant decreased to zero at  $\omega = 8-9$  in the presence of 0.15 mM dissolved organic carbon (DOC) from a water-soil extract. Levels of DOC in natural environments are comparable to the levels found by Inskeep and Bloom (1986) to inhibit calcite precipitation. Lebron and Suarez (1996) incorporated the effect of the DOC in an equation to describe calcite precipitation. This model also includes a term for calcite precipitation by crystal growth and a term for calcite precipitation by heterogeneous nucleation. This is the only model in the literature that attempted to reproduce calcite precipitation in natural environments however, this model was developed only for atmospheric partial pressure of CO<sub>2</sub>. It is well known that concentrations of CO<sub>2</sub> in the root zone are 10-500 times higher than in the atmosphere. With that in mind, the objectives of the present study are: (1) To determine the effect of DOC on crystal growth and heterogeneous nucleation of calcite at different levels of P<sub>CO<sub>2</sub></sub>; and (2) To quantify the effect of P<sub>CO<sub>2</sub></sub> and DOC concentration in a precipitation rate model.

Mineralogical Magazine 62A:864-865, 1999.

# MECHANISMS AND PRECIPITATION RATE OF RHODOCHROSITE AT 25°C AS AFFECTED BY P<sub>CO2</sub> AND ORGANIC LIGANDS

### I. Lebron and D.L. Suarez

Rhodochrosite is the main Mn mineral phase in neutral to alkaline anoxic environments and is likely the initial precipitation phase when Mn<sup>2+</sup> is added to irrigation water. Solutions supersaturated with respect to rhodochrosite that was detected in various natural environments suggest that equilibrium assumptions may not be satisfactory and kinetic processes may be dominant. This study was conducted to evaluate the precipitation mechanisms of rhodochrosite in natural environments where DOC is present and there are variations in partial pressure of  $CO_2$  ( $P_{CO2}$ ). Precipitation rates were measured in supersaturated solutions of rhodochrosite in the presence of seeds of the mineral and P<sub>CO2</sub> 0.035 kPa, 5 kPa, and 10 kPa and in a concentration range of DOC of 0.02 to 3.2 mM of Suwannee River fulvic acid. Precipitation rates were measured in the absence and presence of 1 mM leonardite humic acid. Precipitation rates increased when the P<sub>CO2</sub> increased and decreased when the concentration of the fulvic acid increased at constant levels of supersaturation. However, higher concentrations of DOC were needed to produce the same reduction in precipitation rates when  $P_{\rm CO2}$  was increased. The most likely causes of the increase in the precipitation rate when P<sub>CO2</sub> increases are an increase in the negative surface charge and an increase in the activity of MnHCO<sub>3</sub><sup>+</sup>. No significant change in the precipitation rate of rhodochrosite was measured when the leonardite humic acid was added to the reaction vessels. The lack of inhibition of leonardite humic acid on rhodochrosite precipitation is explained by its molecular configuration in solution.

Soil Sci. Soc. Am. J. 63(3):561-568, 1999.

# SATURATED HYDRAULIC CONDUCTIVITY PREDICTION FROM MICROSCOPIC PORE GEOMETRY MEASUREMENTS AND NEURAL NETWORK ANALYSIS

## I. Lebron, M.G. Schaap and D.L. Suarez

Flow and transport of water and solutes in soils are controlled by the size, geometry and characteristics of the soil porosity. Most of the characteristics of soil pores are microscopic, such as roughness and circularity. Conventional models of liquid distribution, flow and solute transport rely solely on cylindrical capillarity ignoring the role of surface area, angularity, and connectivity. This study was conducted to develop a new methodology to directly measure the porosity and its microscopic characteristics. The methodology is based on the analysis of binary images collected with a backscattered electron detector from thin sections of soils. Pore surface area, perimeter, roughness, circularity, and maximum and average diameter were quantified in 36 thin sections prepared from undisturbed soils. Saturated hydraulic conductivity ( $K_{sat}$ ), particle size distribution, particle density, bulk density and chemical properties were determined on the same cores. We used the Kozeny-Carman equation, neural network and bootstrap analysis to predict a formation factor from microscopic, macroscopic, and chemical data. The predicted  $K_{sat}$  was in excellent agreement with the measured  $K_{sat}$  ( $R^2$ =0.91) when a hydraulic radius defined as  $r_H$  =pore area/pore perimeter and the formation factor were included in the Kozeny-Carman equation.

AGU Conference, vol. 80(46)F370, San Francisco, CA, Abstr., 1999.

### SOIL PORE SPACE AS AFFECTED BY SODIUM

## I. Lebron, D.L. Suarez and M.G. Schaap

Soil porosity and texture are important properties affecting the soil hydraulic properties. Using scanning electron micrographs and image analysis we quantified the actual pore and aggregate size distribution in undisturbed soil cores. We observed, for soils with similar texture, a decrease in the average aggregate size and in the aggregate size distribution when the sodium content in the soil increased and when the pH increased. The cementing agents binding the domains conforming the aggregates were hypothesized to be responsible for the decrease in the aggregate stability. Equivalent decrease in the pore size distribution was found with increasing sodium and pH. There was a significant correlation between average aggregate size and average pore size, but not relationship between average pore diameter and texture. The use of aggregate size distribution instead of soil texture improved the saturated hydraulic conductivity predictions using a pedotransfer function based code.

Agronomy Abstract p. 212, 2000.

## MOBILIZED SOIL CONDUCTIVITY ASSESSMENT SYSTEMS: AN OVERVIEW OF SOME COMMON SYSTEM DESIGN AND DATA INTERPRETATION ISSUES

### S. M. Lesch

Mobilized soil conductivity assessment (MSCA) systems have been used approximately ten years now for the purposes of mapping and monitoring field-scale spatial soil salinity patterns (Rhoades, 1992). More recently, MSCA systems have been increasingly used to map and/or catagorize a wide range of physical/chemical soil properties. This increase in the use and acceptance of such systems is directly related to the current interest in acquiring rapid, accurate precision farming related information. This article presents a brief overview of some pertinent MSCA system design and data interpretation issues. Included here is a review of the basic MSCA system components, some simple system integration concepts, and a general summary of the most commonly used methods for interpreting, modeling, and/or calibrating soil conductivity survey data.

Proceedings 1999 California Plant and Soil Conference. Agricultural Technology - Moving California into the 21st Century. California Chapter of American Society of Agronomy and California Fertilizer Association, 1999.

### THE ESAP-95 VERSION 2.01R USER MANUAL AND TUTORIAL GUIDE

## S.M. Lesch, J.D. Rhoades and D.L. Corwin

This manual describes and documents a series of site selection and salinity modeling software programs, collectively known as the ESAP-95 software package (Release version 2.01R), developed for the analysis and prediction of soil salinity from conductivity survey information. It is designed to be used both as a software reference text and tutorial guide. The ESAP-95 software package currently contains three programs: ESAP-RSSD, ESAP-Calibrate, and ESAP-SaltMapper. The ESAP-RSSD program is designed to generate optimal soil sampling designs from bulk soil electrical conductivity survey information. The ESAP-Calibrate program is design to estimate both stochastic (regression model) and deterministic (soil theory based) calibration equations; i.e., the equations which are ultimately used to predict the spatial values of one or more soil variables from conductivity survey data. The final program, ESAP-SaltMapper, can be used to produce high quality 1D or 2D graphical output of conductivity survey data and/or predicted soil variables. This manual describes and documents the implementation and use of each of these three programs in detail.

George E. Brown Jr. Salinity Laboratory Research Report #146, 2000.

## MODELING ARSENIC (III) ADSORPTION AND HETEROGENEOUS OXIDATION KINETICS IN SOILS

### **B.A.** Manning and D.L. Suarez

Arsenite [As(III)] is a soluble and toxic species of arsenic that can be introduced into soil by geothermal waters, mining activities, irrigation practices, and disposal of industrial wastes. We determined the rates of As(III) adsorption, and subsequent oxidation to arsenate [As(V)], in aerobic soil-water suspensions using four California soils. The rate of As(III) adsorption on the soils was closely dependent on soil properties that reflect the reactivity of mineral surfaces including citratedithionite (CD) extractable metals, soil texture, specific surface area, and pH. Heterogeneous oxidation of As(III) to As(V) was observed in all soils studied. The recovery of As(V) from As(III)treated soils was dependent on levels of oxalate-extractable Mn and soil texture. After derivation of rate equations to describe the changes in soluble and recoverable As(III) and As(V) in soil suspensions, soil property measurements were used to normalize the empirically derived rate constants for three soils. The fourth soil, which had substantially different soil properties from the other three soils, was used to independently test the derived soil property-normalized model. The soil property-normalized consecutive reaction model gave a satisfactory description of the trends seen in the experimental data for all four soils. Understanding the effects of soil properties on the kinetics of chemical reactions of As(III) and As(V) in soils will be essential for development of quantitative models for predicting the mobility of As in the field.

Soil Sci. Soc. Am. J. 64(1):128-137, 2000.

# USE OF EXAFS-DERIVED OXYANION SURFACE STRUCTURES IN A SURFACE COMPLEXATION MODEL

## B.A. Manning, D.L. Suarez and S.E. Fendorf

Oxyanion surface structures derived from extended x-ray absorption fine structure spectroscopy (EXAFS) have been used to constrain the chemical description of the mineral-water interface in a surface complexation model. Arsenic(III) and (V) species were reacted with several synthetic minerals, well-characterized clays, and soil clay fractions followed by EXAFS analysis and wet chemical speciation using high performance liquid chromatography. This approach allowed simultaneous determination of solid-water partitioning data and solid phase analysis. Structural parameters developed in EXAFS data analysis software such as As-Fe and As-Al interatomic distances were then incorporated into the surface complexation model. Data from EXAFS suggested that a suite of adsorption sites (surface site heterogeneity) occurs on crystalline materials and thus extrapolation to soil will require simplifying assumptions.

Agronomy Abstract p. 214, 1999.

# METHODS AND INTERPRETATION OF ELECTRICAL CONDUCTIVITY MEASUREMENTS

### J.D. Rhoades, F. Chanduvi and S.M. Lesch

The technology described in this report for measuring soil salinity has been extensively and successfully field-tested. It is concluded to be sound, reliable, accurate and applicable to a wide variety of useful applications. It is based on proven theory of soil electrical conductivity. The required equipment is commercially available. The advocated instrumental methodology is practical, cost effective and well developed for essentially all general applications. It is cheaper, faster and more informative than traditional methods of salinity measurement based on soil sampling and laboratory analyses. Software is available to facilitate its use for mapping and monitoring uses, as is equipment to mobilize and automate the measurements for use in detailed field-scale assessments. Its usefulness has been demonstrated: 1) for diagnosing soil salinity, 2) for inventorying soil salinity, 3) for monitoring soil salinity, 4) for evaluating the adequacy and appropriateness of irrigation and drainage systems and management practices, 5) for determining the areal sources of excessive leaching, drainage and salt-loading in crop lands, 6) for establishing the spatial soil information needed to develop prescription farming plans to manage fields with spatially-variable salinity conditions, and 7) for scheduling and controlling irrigations under saline conditions. It offers the potential to identify the inherent causes of salinization in fields, especially when integrated with GIS technology, and to identify mitigation needs, especially when integrated with field-scale deterministic, solute transport models. The salinity assessment approach advocated in this report offers a more suitable basis for evaluating, managing and controlling soil salinity than do the leaching requirement and salt balance concepts/measurements as traditionally applied. National programs need to be implemented to mitigate the substantial problems of secondary salinization that threatens the sustainability of irrigation in many places in the world. Holistic; meaningful salinity assessment approaches needed in this regard are illustrated in this report. The presented salinity assessment technology offers substantial practical potential to inventory, monitor, manage and control soil and water salinity, as will be needed to sustain irrigated agriculture and to meet the worlds food needs in the coming decades.

In: FAO Irrigation and Drainage Paper 57, Soil Salinity Assessment, Food & Agriculture Organization of the United Nations, Rome, 1999.

# IMPACT OF AGRICULTURE ON CO<sub>2</sub> FLUXES AS AFFECTED BY CHANGES IN INORGANIC CARBON

### D.L. Suarez

Agricultural practices merit examination for their potential to alter global changes in C fluxes, due to their large impact on the land surface, as well as the large storage of C in soils (about 500 times the net yearly increase in atmospheric CO2 as a result of fossil fuel burning). In this study we examine inorganic C reactions in agricultural soils, including mineral weathering, irrigation of surface and ground waters, liming of acid soils, and application of N fertilizers. Calculations of the impact of these processes for the U.S. and estimation of global effects indicates that although these processes result in net emissions, the effects are less than 1% of the calculated fossil fuel emissions. Potential for changing these C fluxes from inorganic C changes, is relatively low. Assuming to other climatic changes, doubling of the atmospheric CO2 concentration will also have a minor impact on the net inorganic C fluxes from these agricultural processes.

In: R. Lal, J.M. Kimble, H. Eswaran and B.A. Stewart (eds.) "Global Climate Change and Pedogenic Carbonates", Chapter 16, p. 257-272, CRC Press, Boca Raton, FL, 1999.

### TRANSFORMATIONS OF VOLATILE METHYLATED SELENIUM IN SOIL

### D.A. Martens and D.L. Suarez

Microbial volatilization of selenium (Se) as dimethylselenide (DMSe) and dimethyldiselenide (DMDSe) from soil is an important part of the Se cycle in nature, but little is known about the stability and transformations of these gases during residence in the soil environment before dissipation to the atmosphere. Experiments monitored by gas chromatography and atomic absorption spectroscopy were conducted with various clay mineral standards, charcoal, commercial humic substances and soils to determine the sorption and transformations of DMSe and DMDSe injected into the headspace or passed through soil materials. Batch experiments conducted with 2 to 5 g materials placed into 40 mL Teflon centrifuge tubes equipped with MininertTM gas sampling valves showed that DMSe was slowly sorbed by soil materials and the majority of the DMSe deficit in the headspace was recovered as SeO3= and SeO4=. In contrast, DMDSe was rapidly partitioned from the gas phase and resulted in an increased recovery of less soluble elemental and selenide-Se forms. These results were confirmed during flow-through soil column studies with both little DMSe sorption and sorption of the majority of DMDSe addition. Additions of selenomethionine (SeMet) to soil to produce DMSe and DMDSe in sealed flasks resulted in an increased partitioning of Se into inorganic Se when compared with a flow-through system designed to limit the contact of Se gases with soil. These results suggest that soil Se volatilization as DMSe and DMDSe results in Se loss to the atmosphere as DMSe with concomitant soil Se immobilization due to the instability of DMDSe.

Soil Biology & Biochemistry 31:1355-1361, 1999.

### SELENIUM IN WATER MANAGEMENT WETLANDS IN THE SEMI-ARID WEST

### D.A. Martens and D.L. Suarez

The discovery in 1983 of deformities, reproductive failures and high waterfowl mortality rates at Kesterson National Wildlife Refuge, western San Joaquin Valley, CA, due to selenium (Se) contaminated drainage water, raised concerns that these problems may be occurring in the >600 wetlands and National Wildlife Refuges being utilized to collect irrigation drainage waste water in 17 western states. The waterfowl problems were traced to ingestion of organic Se present as Seamino acids. Plants assimilate soluble Se into Se-amino acids and release them upon decomposition. Aerobic plant residue decomposition studies showed that 50% of the assimilated Se was mineralized to soluble Se while the remaining organic Se persisted. This means that each growth cycle results in a steady decrease of soluble Se and an increase in organic Se levels. To test the effect of plant growth on Se accumulation, two types of evaporation ponds were evaluated, one with prolific plant growth and the second, relatively devoid of plant growth. Soil Se analysis showed that plant growth dramatically increased Se accumulation in the surface layers. Evaluation of additional Secontaminated sites showed that Se accumulation followed an exponential function and accumulated rapidly above a 2% soil organic C content. Without plant growth, the Se remains mobile and diffuses to low concentrations in the underlying soil suggesting that plant residue cycling is an important factor in Se accumulation and toxicity.

Symposium: Wetlands and Horticulture: Problems and Solutions. 93rd ASHS Meeting, Lexington, KY, HortScience, 34:34-49, 1999.

## EXTENT, CAUSE AND MANAGEMENT OF SALINITY IN THE U.S.A.

### D.L. Suarez

Increasing demands for high quality water by municipal and industrial users can no longer be met with development of new water supplies in the western U.S. If irrigated agriculture in the western U.S. is to maintain its important role in food production, agriculture will have to utilize lower quality water for irrigation, including reuse of drainage water, use of treated municipal waste waters and development of brackish waters presently considered undesirable for irrigation. The causes of salinity problems in the U.S. are varied, ranging from the presence of saline geologic formations, such as the shales of Colorado and Utah, presence of saline ground water in the upper Great Plains (Dakotas, and north western Colorado) and irrigated areas with either insufficient drainage or non- optimum water management. Salinity problems have been aggravated by excessive rather than insufficient irrigation or infiltration. Increased use of low quality water and implementation of drainage water reuse will require not only improved water management but also application of periodic salinity monitoring and prediction of the impact of management changes on salinity, crop production and soil physical properties. Changes in management practices, such as cyclic reuse of drainage water or supplemental irrigation with low quality waters can now be evaluated using process-based computer models that consider the dynamics of water flow including irrigation amounts and timing, crop water requirements, and sensitivity to water and salt stress, and solution chemistry including the effects of chemistry on soil physical properties. New management practices are needed for minimizing the adverse impact of drainage return flows including toxic anions.

In: Water Reports, Soil Management for Sustainable Use of Salt Affected Soils, Food & Agriculture Organization of the United Nations, (in press) 2000.

# SELENATE AND SELENITE SORPTION ON IRON OXIDES: AN INFRARED AND ELECTROPHORETIC STUDY

#### C. Su and D.L. Suarez

We studied selenate and selenite sorption by amorphous Fe oxide [am-Fe(OH)<sub>3</sub>] and goethite (α-FeOOH) as a function of time (25 min-96 h), pH (3-12), ionic strength (0.01-1.0 M NaCl), and total Se concentration (0.0001-1.0 M). We examined sorbed selenate and selenite by in situ attenuated total reflectance Fourier transform infrared (ATR-FTIR) spectroscopy, diffuse reflectance infrared Fourier transform (DRIFT) spectroscopy, and electrophoresis to deduce sorption mechanisms. Sorption of both selenate and selenite reached equilibrium in <25 min and the sorption isotherm was not reversible. Increasing ionic strength decreased selenate sorption but did not affect selenite sorption. The presence of either selenate or selenite lowered the electrophoretic mobility (EM) and decreased the point of zero charge (PZC) of both sorbents, suggesting inner-sphere complexation for both selenate and selenite species. Both in situ ATR-FTIR and DRIFT difference spectra showed bidentate complexes of selenate with am-Fe(OH)<sub>3</sub>. The structure of selenite complexes in am-Fe(OH)<sub>3</sub>- solution interface was uncertain due to insensitivity of the in situ ATR-FTIR technique. The DRIFT spectra of selenite on am-Fe(OH)<sub>3</sub> showed  $v_3$  splitting as evidence of complexation. The DRIFT spectra of selenite on goethite showed bridging bidentate complex of selenite. We conclude that the influence of ionic strength on Se sorption cannot be used as a criterion for distinguishing outer- vs. inner-sphere complex formation.

Soil Sci. Soc. Am. J. 64(1):101-111, 2000.

### THE FUTURE OF SOIL MANAGEMENT FOR SALINITY CONTROL

### D.L. Suarez

Increasing competition for scare water resources will result in the use of lower quality water for irrigation. There is also increased environmental concern about off-site impacts of drainage waters. These factors result in increased salinity hazard thus the need to improve management. Evaluation of salinity status is possible with rapid EM measurements in combination with GPS information and GIS for rapid signal processing and display of results. Improved evaluation of management options will be possible with development of user friendly computer simulation models that are compatible with the type and data structure of the sensing equipment, and that incorporate the detailed processes of water distribution, infiltration and transport, chemical reactions and plant water uptake and growth. Such integrated tools will allow us to utilize precision farming concepts for salinity management, taking into account the spatial variation in soil properties, salinity and chemistry and improving water distribution while minimizing drainage return flows.

Agronomy Abstract p. 285, 1999.

# IMPACT OF IRRIGATED AGRICULTURE ON SOIL CARBON STORAGE IN COLORADO RIVER BASIN

### D.L. Suarez

Agricultural practices may result in both addition or removal of inorganic and organic carbon from soils. Interest in characterizing changes in inorganic carbon as a result of irrigation stem from both the large quantities of inorganic carbon in soils as well as model calculations suggesting large amounts of carbonate precipitation. Soil cores were taken from Grand Valley, Palo Verde Valley and Imperial Valley, all irrigated with Colorado River water for up to 110 y. Matched cores (irrigated and never irrigated) were taken from adjacent locations. Samples were analyzed with depth for soil texture, inorganic carbon, organic carbon and carbon isotopic composition. Analysis of these cores indicated no significant differences in the inorganic carbon and minor differences in the organic carbon content of the irrigated and adjacent non-irrigated soils. Consistent with these results, the stable C isotopic analyses indicated that almost all the carbonate was of marine origin. The slightly lighter 12 C/13 C isotopic ratio in some of the irrigated sites is consistent with minor amounts of reprecipitated calcite as a result of wetting and drying cycles associated with irrigation practices. These data are not consistent with steady state models of carbonate precipitation based on estimated leaching fractions, that predict large increases in inorganic carbon storage as a result of irrigation in the lower Colorado River basin. Experimental data were also compared to results from simulations using the UNSATCHEM model. Consideration of the dynamics of CO<sub>2</sub> root zone transport and concentrations, calcite precipitation kinetics and additions of NH<sub>4</sub> fertilizers suggest that limited precipitation may occur lower in the soil profile. Mass balance calculations based on alkalinity in irrigation and drainage water are consistent with inorganic carbon precipitation. Additional measurements in these and other basins, including deeper subsurface samples are needed to quantify the impact of irrigation on carbon storage in semi-arid and arid lands.

Advances in Terrestrial Ecosystem Carbon Inventory, Measurements, and Monitoring, Raleigh, NC, Abstr., 2000.

# MODELING IRRIGATION WITH LOW QUALITY WATERS AND SODIC SOIL RECLAMATION

### D.L. Suarez

Existing water quality criteria for irrigation consider salinity and the sodium adsorption ratio. These parameters reflect the adverse effect of Na (and low salinity) on soil hydraulic properties, but do not consider the infiltration rates required for specific crop and climatic conditions nor the achievable infiltration rates under actual field conditions. Similarly, chemical transport models that consider plant water uptake have been utilized for predicting the long term effects of irrigation on chemical parameters, but the effects on hydraulic characteristics have not been incorporated into these models. The UNSATCHEM model has unique capabilities including CO<sub>2</sub> production and transport routines for dynamic prediction of pH as well as consideration of the effects of chemical properties, including pH, on soil hydraulic characteristics and infiltration. Soil and managementspecific information is required to enable simulation of the site-specific conditions. Examples of the use of the model are provided from field and laboratory studies of sodic soils from Coachella, CA. Simulations of irrigation on sodic soils illustrates the importance of soil texture and related hydraulic and chemical properties on ease of reclamation. Reclamation schemes can be evaluated in terms of amounts of amendments, water and time required for restoration of adequate infiltration. Similarly irrigation with low quality water may not result in immediate adverse effects on infiltration and salinity but long term effects may be very adverse. Since long term effects are not easily measured experimentally, there is need for conceptual understanding of the processes and subsequent model simulation of the time-dependent processes.

Sodicity Issues in Agricultural Industries-Current Research and Future Directions, in Tatura, Victoria, Australia, Abstr., 2000.

# UNSATCHEM3.0 WATER AND MULTICOMPONENT CHEMICAL TRANSPORT WITH WINDOWS USER INTERFACE

### D. L. Suarez, P.J. Vaughan and S.M. Lesch

The UNSATCHEM model has been updated with inclusion of additional chemical capability, conversion to 32 bit double precision code and a Windows based interface. The interface consists of a pre and post processor with graphing capability. In addition to the previous capabilities to predict CO2 production and transport, variably saturated water flow, heat flow major ion cation exchange and precipitation-dissolution of calcite, gypsum and Mg carbonates, the model now includes consideration of calcite precipitation kinetics including the inhibiting effect of DOC on precipitation, capability to consider multisite cation adsorption, enabling prediction of cation selectivity based on organic matter and clay mineral content, B chemistry and adsorption using the constant capacitance model, silicate mineral weathering, including feldspars, micas and hornblende, and calculation of  $\text{Et}_c$  using crop coefficients and the Penman Monteith equation. The model is freely available and includes a user manual.

Agronomy Abstract p. 41, 2000.

### PREDICTION OF B TRANSPORT IN SOIL COLUMNS

#### D.L. Suarez

Reuse of agricultural and municipal waste waters are often limited by the elevated concentrations of B. Use of these water requires ability to predict the B concentration in solution with time, as well as development of effective reclamation practices. Existing B transport models require detailed soil-specific B adsorption-desorption characterization or empirical fitting of  $K_d$  parameters. This study compares the predictive capability of the UNSATCHEM model utilizing surface area to estimate the surface site density (moles/g) and generalized constant capacitance parameters. Three arid land soils were packed into soil columns, reacted with 0.08 mmol/L B solutions at pH 6 and pH 9, and subsequently leached with pH 6 and 9, B- free water. At elevated pH B adsorption increased and desorption was decreased relative to pH 6. The model was able to adequately predict B concentrations during both adsorption and desorption without the need to characterize the sorption characteristics of each soil. The greatest uncertainty in predicting B concentrations was associated with fluctuations in soil pH.

Agronomy Abstract p. 230, 2000.

### ROLE OF GROUNDWATER FLOW IN TILE DRAIN DISCHARGE

## P.J. Vaughan, D.L. Suarez, J. Šimůnek, D.L. Corwin and J.D. Rhoades

Tile systems drain water applied to agricultural fields as irrigation and precipitation but also may intercept regional groundwater flow. Identification and characterization of the potential sources of tile water is essential for informed management of salinity and contaminants. Factors influencing tile discharge including depth of water applied, evapotranspiration, water storage, drain blockage, and interception of regional groundwater flow were evaluated to determine which may be related to a fivefold variation in cumulative tile discharge among six sumps located 100 km west of Fresno, CA. Cumulative depths drained were calculated for 5 yr of weekly irrigation, precipitation, and discharge data. Evapotranspiration and water storage were estimated using the UnsatchemGeo variably-saturated water flow model. Well water levels measured on 19 dates were spatiallyaveraged providing spatial variation of depth-to-water among the drained areas. Variability in depth of water drained (0.18-0.95 m) was large and was not correlated with either water applied (3.26-4.58 m,  $r^2$ =0.03) or with computed water flux from the bottom of the soil column (0.05-0.31 m,  $r^2$ =0.00). Groundwater interception by tile drains was a factor because depth-to-water was negatively correlated with discharge ( $r^2$ =0.42) and drawdown of groundwater levels by drains was relatively larger for those drained areas encountered first during regional groundwater flow. For all six sumps, drained water is likely derived from locally applied water and interception of regional groundwater flow implying that standard two-dimensional models of flow to drains, representing only water applied locally, would not be applicable to modeling of drain flows or drain-water solute concentrations.

J. Environ. Qual. 28(2):403-410, 1999.

### ABOVE-CANOPY CO<sub>2</sub> FLUX FOR WHEAT IN CENTRAL OKLAHOMA: A COMPARISON OF MODEL RESULTS WITH MEASURED DATA

### P.J. Vaughan and D.L. Suarez

At AmeriFlux sites CO2 flux is measured continuously to provide information about the processes and extent of carbon sequestration in the soil in different ecosystems. A data set consisting of meteorological measurements made every half-hour at a height of 4.5 m at the AmeriFlux Wheat Site in Oklahoma was processed to remove all gaps in the data to prepare it for modeling. The 1-D Unsatchem model was linked to the GAS-FLUX layered canopy gas exchange model to make the USGF combined model. Photosynthesis model parameters for canopy gas exchange were published values of single-leaf gas exchange in wheat. Parameter values for the subsurface CO<sub>2</sub> production model were the same as those used in earlier modeling of soil surface CO<sub>2</sub> flux in wheat by Unsatchem. When the scaling constants for photosynthesis in light-saturated and light-limited conditions were adjusted to optimal value, predictions of CO<sub>2</sub> flux matched measured flux. The Wheat site was located within the ARM-CART SGP97 area, the wheat-growing areas were classified by the SGP97 project. A subarea surrounding the Wheat site was selected for estimation of daily net carbon balance occurring in wheat. The calculation indicated net CO<sub>2</sub> loss in this area during 1996-97 but uncertainty suggests that making CO<sub>2</sub> surface flux measurements could provide additional constraints on the subsurface CO<sub>2</sub> production.

4th International Conference on Integrating GIS & Environmental Modeling (GIS/EM4), Available at the following web site: <a href="http://www.Colorado.edu/research/cires/banff/upload/75">http://www.Colorado.edu/research/cires/banff/upload/75</a>, 2000.

## ATMOSPHERIC CO2 FLUX PREDICTION BY USGF MODEL FOR AMERIFLUX WHEAT SITE

### P.J. Vaughan, R.J. Ryel, D.L. Suarez and C.W. Rice

The Unsatchem model of water flow, CO<sub>2</sub> transport and multicomponent solute transport in the vadose zone was linked to the GAS-FLUX canopy photosynthesis and transpiration model to generate the USGF model of combined plant and soil processes. Linkage includes feedback of the mean water pressure head within the root zone to the plant model through reduction of the maximum stomatal conductance by a water stress factor. Transpiration calculated in the GAS-FLUX component determines root water uptake. Data required by USGF include solar radiation, precipitation, weather data, photosynthesis model parameters and plant structure such as LAI and leaf angles for different levels in the canopy. Predictions include water and CO<sub>2</sub> flux above the canopy. Data collected at the Ameriflux Wheat site (OK) during 9/96-8/97 at 30-minute intervals are sufficiently detailed for comparison of model results with measured flux data.

Agronomy Abstract p. 15, 1999.

# NET ECOSYSTEM EXCHANGE CALCULATED FOR THE AMERIFLUX WHEAT SITE, OKLAHOMA

### P.J. Vaughan and D.L. Suarez

Net ecosystem exchange measured at the AmeriFlux Wheat Site in Oklahoma by the eddy covariance technique was compared to model results obtained from the USGF combined model of canopy gas exchange and subsurface CO2 production and transport. The simulations were run for a 352-day period in 1996-97 that overlaps the winter wheat growing season. The advantage of using CO2 flux to calculate carbon storage instead of simply measuring the changes in soil carbon concentration is that the length of the simulation required for calculating a meaningful change in carbon storage is much shorter. Preliminary results suggest that there was a small loss of carbon from the subsurface during the 352-day period. These simulations suggest that measurement of CO2 surface flux could provide a useful complement to above-canopy CO2 flux enabling more accurate parameterization of the subsurface CO2 production and transport model. Application of the model to various ecosystems is possible and desirable because the model could be used for making spatial predictions of carbon sequestration that, being based on calculation of carbon flux, would provide a sensitive estimation as compared to a carbon-pool type of model.

Advances in Terrestrial Ecosystem Carbon Inventory, Measurements, and Monitoring. Raleigh, NC, Abstr., 2000.

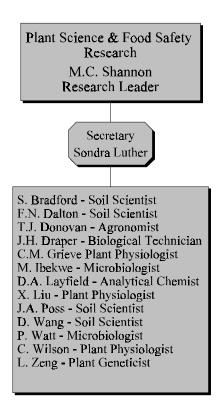
## PARAMETERIZATION OF LINKED CANOPY GAS EXCHANGE AND SOIL PROCESS MODEL

### P.J. Vaughan

Atmospheric CO2 flux, measured at the AmeriFlux Wheat Site in Oklahoma, was compared to predictions of above-canopy flux by a linked model of canopy gas exchange and subsurface CO2 production and transport. A standard error of the estimate (sigma) was computed for year-long simulations utilizing different sets of model parameter values. Calculation of net photosynthesis in the canopy gas exchange model required calculation of Vcmax, the maximum carboxylation rate, and Pml, the CO2- and light-saturated rate of photosynthesis. By varying the scaling factors (Fvc and C) in the Johnson-Eyring expressions for these two rates, a surface representing sigma on a plot of Fvc vs. C was found to have two orthogonal minimum branches. This shape occurred because the modeled light-response curve had nearly the same form for different (Fvc,C) pairs along the minimum in sigma. Other parameters that were studied include the activation energy and scaling factor for dark respiration, quantum efficiency, and leaf angle.

Agronomy Abstract p. 28, 2000.

# Plant Science & Food Safety Research



### Mission

The mission of the Plant Science & Food Safety Research unit is to increase the yields, quality, safety, and desirability of agronomic and horticultural plants grown on salt affected soils. The unit is charged with evaluating the tolerance of plant species, developing an understanding of the interactive effects of salinity and environmental factors on plants, elucidating the morphological, biophysical, biochemical and molecular mechanisms of salt tolerance and salt injury, developing a basis for genetic increases in salt tolerance, and developing control strategies to prevent transmission of pathogens from animal waste operations to food-producing animals, agricultural crops, surface and ground waters. These principles are to be integrated into crop response models, and soil/water transport models which can be used to recommend management practices and systems that improve agricultural productivity, food safety, and environmental protection.

### PLANT SCIENCE & FOOD SAFETY RESEARCH STAFF



### MICHAEL C. SHANNON, B.S., Ph.D., Laboratory Director, Supervisory Research Geneticist for Plant Science & Food Safety Research

Genetic screening for crop Tolerance to soil salinity; heritable characteristics of plant uptake and exclusion-of ions for soils and irrigation waters

# CATHERINE M. GRIEVE, B.S., Ph.D., Plant Physiologist for Plant Science & Food Safety Research.

Effect of water quality on morphological development of small grain crops. Plant response to irrigation water composition. Identification of halophytic crops for drainage water reuse systems.





# CLYDE WILSON, B. A., M. S., Ph. D., Research Plant Physiologist for Plant Science & Food Safety Research.

Biochemical and biophysical mechanisms underlying adaptaion to saline environments; photosynthetic and stomatal responses to saline irrigation water; bioenergetic and membrane changes due to salt stress.

# DONG WANG, B.S., M.S., Ph.D., E.I.T., Soil Scientist for Plant Science & Food Safety Research.

Drip, sprinkler, furrow irrigation systems; processes and mechanisms attributing to soil and water salinity; environmental biophysical factors affecting plant growth under saline environment; heat and mass transfer in the soil-water-plant-atmosphere continuum.



### PLANT SCIENCE & FOOD SAFETY RESEARCH STAFF



# FRANCIS N. DALTON, B.S., M.S., Ph.D., Research Soil Scientist for Plant Science & Food Safety Research.

Simulation of coupled water and ion uptake by plant roots as it relates to plant response in saline environments; development of environmentally independent dynamic salinity stress index, SSI, Instrumental techniques for in-situ measurement of soil water content/electrical conductivity; soil/plant water energetics, root extent/distribution.

# A. MARK IBEKWE, B.S., M.S., Ph.D., Research Microbiologist for Plant Science & Food Safety Research.

Detection, survival, transport, and reduction of human pathogens in the environment. Primary research focus in the area of Plant-Microbe interactions and the role of microorganisms in the ability of soil to recover from degradation after disturbance or response to stress.





# SCOTT BRADFORD, B.S., M.S., Ph.D., Soil Scientist for Plant Science & Food Safety Research.

Detection, survival, transport, and reduction of human pathogens in the environment. Multiphase flow and transport of organic and inorganic contaminants in soil and aquifer systems.

# MICROPORE PROCESSES, MEASUREMENTS AND MODELS RELATED TO ROOT WATER EXTRACTION AND PLANT RESPONSE IN SALINE ENVIRONMENTS

#### F.N. Dalton

The ability to correlate the dynamic behavior of macroscopic properties of a soil-plant system in terms of fundamental micropore processes provides significant insights to the predominant physical phenomena governing plant response in saline environments. This paper shows that with respect to salinity, the onset of yield reduction is fundamentally related to the dynamics pore water ion transport to root xylem tissue and not, as it traditionally assumed, to the osmotic potential of the pore water. Besides micropore processes and biophysical transport properties of roots, ion transport is shown to be controlled by climatic variables that simultaneously effect water use and growth. Concepts to be revisited include the significance of the relative root surface area that is in contact with liquid phase pore water and why matric and osmotic potentials cannot be assumed to be additive with respect to yield reduction.

Agronomy Abstract p. 174, 1999.

#### CROP RESPONSE AND MANAGEMENT OF SALT-AFFECTED SOILS

### L.E. Francois† and E.V. Maas

Salinity is a major factor reducing plant growth and productivity throughout the world. Approximately 10% of the world's 7 x 10<sup>9</sup> ha arable land surface consists of saline or sodic soils. The percentage of cultivated lands affected by salts is even greater. Of the 1.5 x 10<sup>9</sup> ha cultivated lands, 23% are sonsidered saline and another 37% are sodic. Although the data are tenuous, it has been estimated that one-half of all irrigated lands (about 2.5 x 10<sup>8</sup> ha) are seriously affected by salinity or waterlogging. Historically, soil salinity contributed to the decline of several ancient civilizations. Despite the advanced management technologies available today, salinization of millions of hectares of land continues to reduce crop production severely in the United States and worldwide. The National Academy of Sciences includes salinization of soils and waters as one of the leading processes contributing to a world-wide biooogical catastrophe.

Sustained and profitable production of crops on salt-affected soils is possible if appropriate onfarm management decisions are made. To be successful, growers require an understanding of how plants respond to salinity, the relative tolerances of different crops and their sensitivity at different stages of growth, and how different soil and environment conditions affected salt-stressed plants. This chapter discusses the effect of soil and water salinity on agronomic and horticultural crop plants, presents data on the tolerance of crops to salinity, and considers consequences of various cultural and management practices on crop yield responses.

In: Handbook of Plant and Crop Stress (M. Pessarakli, Ed.), Marcel Kekker, Inc., New York, Chapt. 8, pgs 169-201, 1999.

† Deceased

#### SCREENING EUCALYPTUS CLONES FOR SALT TOLERANCE

### C.M. Grieve, M.R. Guzy, J.A. Poss and M.C. Shannon

Agroforestry plantations offer environmentally-acceptable strategies for the reuse of saline drainage waters. Tree species suitable for use in such systems must be selected for survival and sustained growth under highly saline conditions. In this screening trial, four clones of Eucalyptus camaldulensis Dehn. (4543, 4544, 4573, and 4590) and one clone of E. rudis Endl. (4501) were grown in greenhouse sand cultures irrigated with sodium sulfate-dominated waters. Solution compositions were prepared to simulate saline drainage waters typically found in the San Joaquin Valley of California. Electrical conductivities of the solutions ranged from 2 to 28 dS m<sup>-1</sup>. Treatments were replicated three times. All plants survived and were harvested after 7 weeks under saline treatment. Plant height was measured weekly and shoot biomass was determined at final harvest. The salinity levels that resulted in a 50% reduction in biomass production (C<sub>50</sub>) were 16.4 (4573), 17.1 (4543), 17.7 (4544), 29.0 (4590), and 30.0 dS m<sup>-1</sup> (4501). Over the range of salinities from 4 to 20 dS m<sup>-1</sup>, clones 4501, 4590, and 4573 generally maintained higher relative growth rates (RGR) than did clones 4544 and 4543. However, at the highest salinity, RGR of clones 4501, 4544 and 4573 were significantly greater than those of clones 4543 and 4590. Assessed on the basis of biomass production, clones 4501 (E. rudis) and 4590 (E. camaldulensis) showed exceptional potential for use in agroforestry systems where the saline drainage waters are sodium sulfate-dominated.

HortScience 34:867-870, 1999.

# SALINITY EFFECTS ON GROWTH, SHOOT-ION RELATIONS, AND SEED PRODUCTION OF LESQUERELLA FENDLERI

### C.M. Grieve, M.C. Shannon and D.A. Dierig

Lesquerella [Lesquerella fendleri (Gray) S. Wats.] was grown in outdoor sand cultures irrigated with waters designed to simulate saline drainage effluents present in the San Joaquin Valley of California, and compositions that would result from further concentration of the water. These waters are typically high in Na<sup>+</sup>, SO<sub>4</sub><sup>2-</sup>, Cl<sup>-</sup>, Mg<sup>2+</sup>, and Ca<sup>2+</sup>, predominating in that order. Salts were added to complete nutrient solutions to give eight salinity treatments with electrical conductivities (EC) of 3, 6, 9, 12, 15, 18, 21, and 24 dS·m<sup>-1</sup>. Treatments were replicated three times. Vegetative growth, seed yield, leaf- and stem-ion content were determined. Plant survival was reduced when salinity exceed 15 dS·m<sup>-1</sup> and continued to decrease over time. The few survivors in the 24 dS·m<sup>-1</sup> treatment were rescued and eventually grown in crossing blocks under nonsaline conditions. The divalent cations, Ca<sup>2+</sup> and Mg<sup>2+</sup>, were strongly accumulated in the shoots and were preferentially partitioned to the leaves rather than the stems. Chloride partitioning followed a similar pattern. In contrast, Na<sup>+</sup> and K<sup>+</sup> were more uniformly distributed between leaf and stem tissues. Leaf-Ca and-K decreased with increasing salinity, whereas leaf-Na and -Cl increased. Biomass production was reduced by 50% at 14.9 dS·m<sup>-1</sup>. Leaf area decreased consistently from a mean of 950 to 65 cm<sup>2</sup> per plant as irrigation water salinity increased from 3 to 21 dS·m<sup>-1</sup>. Average seed yield per plant was ~2 g in the 3, 6, 9, and 18 dS·m<sup>-1</sup> treatments and 3 g at 12 and 15 dS·m<sup>-1</sup>.

Book: IN: J. Janick (ed.), Perspectives on New Crops and New Uses, Part III, p. 239-243, ASHS Press, 1999. Proc. 4th Nat'l. Symp., AAIC, "New Crops and New Uses Biodiversity and Agricultural Sustainability, Phoenix, AZ, Nov. 8-11, 1998.

# ION ACCUMULATION AND DISTRIBUTION IN SHOOT COMPONENTS OF SALT-STRESSED EUCALYPTUS CLONES

#### C.M. Grieve and M.C. Shannon

Four clones of Eucalyptus camaldulensis Dehn. (4543, 4544, 4573, and 4590) and one clone of E. rudis Endl. (4501) were grown in greenhouse sand cultures irrigated with sodium-sulfate dominated waters. Electrical conductivities of the solutions were 2, 12, and 28 dS m<sup>-1</sup>. Treatments were replicated three times. Mechanisms of differential salt tolerance based on ion uptake and distribution patterns in above-ground components were studied in saplings grown under treatment for 7 weeks. Potassium and Mg<sup>2+</sup> were preferentially accumulated in the youngest leaves in the upper portion of the canopy, whereas Ca<sup>2+</sup> was retained in the older leaves. At the lowest salinity level, phosphorus was translocated to the youngest leaves, but was more uniformly distributed in the canopy as salinity increased. Leaf- and stem-Cl levels tended to be higher in all clones grown at 2 dS m<sup>-1</sup> than at 28 dS m<sup>-1</sup>. The clones could be separated into two distinct groups by significant differences in leafion relations and, to a lesser degree, stem-ion content. Group 1, clones 4543, 4544, and 4573, were more active Na<sup>+</sup>-excluders and accumulated more Ca<sup>2+</sup> and Cl<sup>-</sup> than clones 4501 and 4590. Clones in group 2, 4501 and 4590, were relatively active Na<sup>+</sup>accumulators under low salinity, but apparently possessed some mechanism for restricting leaf-Na<sup>+</sup> that was activated as salinity increased. In response to the 28 dS m<sup>-1</sup> treatment, the efficiency of K<sup>+</sup> uptake relative to Na<sup>+</sup> by both groups was unusually high. At this salinity level, mean K<sup>+</sup>: Na<sup>+</sup> selectivity coefficients were 315 and 130 for the leaves of clones of groups 1 and 2, respectively.

Amer. Soc. Hort. Sci. 124:559-563, 1999.

# EFFECT OF SALINE IRRIGATION WATER COMPOSITION ON SELENIUM ACCUMULATION BY WHEAT

### C.M. Grieve, D.L. Suarez and M.C. Shannon

Trace amounts of selenium are essential for animal and human nutrition. However, the optimum concentration range is very narrow and outside of this range deficiencies or toxicities can occur. Potentially harmful levels of selenium in soils and irrigation waters have been reported in regions where salinity is also a hazard. This study was conducted to determine the effects of irrigation water composition and salinity level on selenium accumulation in leaves and grain of spring wheat (Triticum aestivum L. cv. 'Yecora Rojo'). Plants were grown in greenhouse sand cultures and irrigated with complete nutrient solution. Salinity treatments were initiated 4 days after planting by irrigating the seedlings with either chloride-dominated waters or with waters containing both chloride and sulfate salts. Compositions of the mixed salt waters were designed to simulate saline drainage waters commonly present in the San Joaquin Valley of California. The experimental design was a randomized complete block with two salinity types (Cl or mixed salts), eight salinity levels (osmotic potentials = 0.07, 0.16, 0.21, 0.30, 0.36, 0.44, 0.52, and 0.63 MPa), and three replications. Four weeks after planting. Se (1 mg L<sup>-1</sup> as sodium selenate) was added to all irrigation waters. In the chloride system, the molar ratio of  $SO_4^{2-}$ :  $SeO_4^{2-}$  was approximately 110 across all salinity levels, whereas in the mixed salt system, the SO<sub>4</sub><sup>2</sup>-:SeO<sub>4</sub><sup>2</sup>- ratio in solution increased from about 300 to 4700 as salinity increased. Selenium concentration was determined in fully-expanded flag leaf blades and grain. Salinity type, and to a lesser extent, salinity affected Se accumulation. In the Cl<sup>-</sup>-system, wheat accumulated Se to levels that may be potentially harmful to livestock and humans, e. g. blade-Se ranged from 435 to 295 mg kg<sup>-1</sup> dry wt; grain-Se ranged from 81 to 54 mg kg<sup>-1</sup> dry wt. Under the saline conditions of the mixed salt system, the inhibition of selenium uptake by sulfate reduced both blade- and grain-Se to levels that would minimize the health risk to consumers.

J. Plant Nutrition, 22:1443-1450, 1999.

#### WHEAT RESPONSE TO INTERACTIVE EFFECTS OF BORON AND SALINITY

#### C.M. Grieve and J.A. Poss

In semiarid regions with irrigated agriculture, excess boron (B) often occurs in association with moderate to high salinity. However, little information is available on plant uptake of B under saline conditions. This greenhouse study was conducted to determine the interactive effects of salinity and varying concentrations of boron on growth, yield and ion relations of wheat (Triticum aestivum L., cv. 'Yecora Rojo'). Plants were grown in sand cultures that were irrigated four times daily with modified Hoagland's nutrient solution. Sixteen treatments were initiated 4 d after planting in a completely randomized factorial experiment with 4 salinity levels (electrical conductivities of the irrigation waters = 1.5, 4, 8, and 12 dS  $m^{-1}$ ) and 4 B concentrations (1, 5, 10, and 15 mg  $L^{-1}$ ). Salinizing salts were NaCl and CaCl<sub>2</sub> (2:1 molar basis). Symptoms of B toxicity were closely correlated with B concentration in the leaves and injury became severe when leaf-B exceeded 400 mg kg<sup>-1</sup>. At each concentration of external B, shoot-B was least under nonsaline conditions and increased significantly as salinity increased. Shoot-calcium (Ca) concentration increased with increasing salinity, but was unaffected by applied B. Shoot-magnesium (mg), and potassium (-K) decreased significantly in response to increases in salinity and substrate B. Salinity and B as well as their combined effects significantly reduced wheat biomass production, yield components, and final grain yield.

J. Plant Nutr. 23: 1217-1226, 2000.

#### SALT TOLERANCE OF VEGETABLES

#### C.M. Grieve

In the near future, the challenge to growers, irrigation specialists, and horticultural scientists will be to maintain the high quality and wide variety of vegetables presently available to consumers in spite of constraints on fresh water supplies. High quality irrigation waters allocated for agriculture are threatened by increased competition from urban users. As an alternative, strategies for on-farm reuse of saline drainage water are under development, particularly in those areas that lack sufficient drainage outlets. Vegetable crops are, in general, moderately sensitive to salinity. A notable exception is asparagus (*Asparagus officinalis* L.) which is rated as the most salt tolerant vegetable crop. Other moderately salt tolerant crops are Swiss chard and garden beet (*Beta vulgaris* L.), turnip greens (*Brassica rapa* L. Rapifera Group), and purslane (*Portulaca oleracea* L.). Salinity-related nutritional disorders may result in cause leaf damage that reduce quality and marketability. Vegetable species have a reasonable capacity for high growth under low to moderate saline conditions. If, however, these crops are to have market potential, irrigation practices must be closely managed to control soil salinity within acceptable levels.

Irrigation J. 50:28-30, 2000.

# EFFECT OF SALINE IRRIGATION WATER COMPOSITION ON GROWTH, SHOOT ION RELATIONS AND SELENIUM UPTAKE BY LESQUERELLA FENDLERI (GRAY) S. WATS

C.M. Grieve, J.A. Poss, D.L. Suarez and D.A. Dierig

This study was conducted at the U.S. Salinity Laboratory, Riverside, CA to compare the response of lesquerella to irrigations waters differing in composition, namely, Cl-dominated salinity (NaCl:CaCl<sub>2</sub>, 2:1 molar ratio), and mixed slat salinity (Na, So<sub>4</sub>, Mg, and Cl as the predominant ions). The Cl-system has been used extensively in evaluation of salt tolerance of various crops, whereas the mixed salt-system is typical of saline drainage waters commonly encountered in the San Joaquin Valley of California. A further objective of the study was to determine the uptake of selenium by lesquerella irrigated with saline waters contaminated with this potentially toxic trace element.

Lesquerella was direct-seeded in 24 greenhouse sand tanks and irrigated with complete solutions. Salinity was imposed one month after planting; twelve tanks were irrigated with Cl-based waters and 12 with mixed salt salinity. The solutions were isoosmotic at each salt level: 0.070, 016, 0.30 and 0.52 MPa, with electrical conductivities (EC<sub>i</sub>) of approximately 1.7, 4.8 and 12 dS•m<sup>-1</sup>, respectively. One month later, selenium (1 mg•L<sup>-1</sup>, 12.7 μM) was added to all solutions as Na<sub>2</sub>SeO<sub>4</sub>.

Regardless of salinity type, shoot biomass production was not significantly reduced until  $EC_i$  exceeded 8 d dS•m<sup>-1</sup>. At 12 dS•m<sup>-1</sup>, shoot dry weight decreased 60% in response to chloride-salinity and 40% in the mixed salt system.

Leaf tissue contained higher concentrations of Ca, Mg, Cl, S, and Se, than the stems; whereas concentrations of the monovalent cations, Na and K were higher in the stems than the leaves. Salt-stressed lesquerella shoots contained relatively low concentrations of Na and K compared to other cruciferous plants. In both salinity systems, the calcicolous nature of lesquerella was expressed by strong accumulation of Ca by both leaves and stems.

Selenium accumulation by lesquerella shoots was strongly influenced by the composition of the external media. In response to irrigation with Cl-dominated solutions, leaf-Se (mean = 500 mg•kg¹) tended to decrease with increasing salinity, but this effect was not statistically significant. In contrast, the competitive inhibition of Se uptake by increasing concentrations of SO<sub>4</sub> was evident in lesquerella irrigated with waters prepared to simulate San Joaquin Valley drainage effluents. Leaf-Se decreased from 220 to 13 mg•kg¹¹ as in salinity increased from 1.7 to 12 dS•m¹¹. Based on these preliminary results, lesquerella should be further evaluated as a potentially useful crop for the phytoremediation of Se-contaminated saline soils particularly in those systems where the dominant anion is Cl.

Proc. Assoc. Advancement Ind. Crops, "Diversity in Agricultural Products: New Crops and New Markets, Eugene, OR., Abstr. Pg. 28, Oct. 17-21, 1999.

## SALINITY AND IRRIGATION METHOD AFFECT MINERAL ION RELATIONS IN SOYBEANS

### C. M. Grieve, D. Wang and M.C. Shannon

Soybean (*Glycine max* (L.) Merrill) is moderately salt tolerant, but the method of irrigation used for crop production under saline conditions may influence the uptake of potentially toxic salts. This field study was conducted to determine the effects of application of saline waters by drip or above-canopy sprinkler irrigation on ion relations of the soybean cultivar 'Manokin'. Salinity was imposed by adding NaCl and CaCl<sub>2</sub> to nonsaline irrigation waters. Saline treatments with electrical conductivities (EC<sub>i</sub>) of 4 dS·m<sup>-1</sup> were compared with nonsaline controls (EC<sub>i</sub> = 0.5 dS·m<sup>-1</sup>). Ion concentrations in leaves, stems, roots, and, when present, pods were determined at four stages of growth: vegetative, flowering, podding, and grain filling. In response to saline drip irrigation, Na<sup>+</sup> and Cl<sup>-</sup> were retained in the basal parts of the plant with only limited partitioning of these ions to the leaves. Leaf-Na and -Cl concentrations in plants drip irrigated with saline water were 3 and 28 mmol·kg<sup>-1</sup>, respectively, at the grain-filling stage. When saline water was applied by over-canopy sprinkling, concentrations of Na<sup>+</sup> and Cl<sup>-</sup> in the leaves were about 9-fold higher than in plants under saline drip irrigation. Regardless of treatment, leaf-K was highest during the vegetative stage of development, and then decreased with plant age as K<sup>+</sup> was mobilized to meet the nutrient demands of the developing reproductive structures.

Agronomy Abstract p. 116, 2000.

#### DETECTION OF E. COLI 0157:H7 IN ENVIRONMENTAL SAMPLES

#### A.M. Ibekwe and M.C. Shannon

Enteric infections due to food-borne bacterial pathogens account for annual losses of 3.5 billion dollars in the US. Detection of *Escherichia coli* 0157:H7 and other enterohemorrhagic serotypes (EHEC) in environmental samples is particularly challenging. *Escherichia coli* 0157:H7 is commonly carried by healthy cattle and shed in their feces. Cross-contamination of fruits and vegetables with manure or improperly composted manure are potential sources of pathogen contamination during preharvest. In this study we developed and evaluated the use of multiplex PCR method that rapidly detects EHEC 0157:H7 in environmental samples. Animal manure collected from a commercial dairy operation were inoculated with the pathogen and cultured in a modified-GN broth overnight. DNA was extracted and used in a multiplex PCR assay to amplify a 150 bp fragment of the virulence genes eaeA of EHEC 0157-H7. With this method we detected 10 to 100 cfu of EHEC after overnight growth in a single enrichment.

Agronomy Abstract p. 398, 2000.

## CARBON ISOTOPE DISCRIMINATION AND TRANSPIRATION EFFICIENCY IN EUCALYPTUS UNDER SALINITY AND BORON STRESS

J.A. Poss, S.R. Grattan, D.L. Suarez, C.M. Grieve and M.C. Shannon

We tested the hypothesis that stable carbon-isotopic composition in Eucalyptus trees can be an indicator of the cumulative salinity and boron stress history of the plant. In a controlled, outdoor sand-tank study, Eucalyptus camaldulensis saplings were irrigated with combinations of salinity (EC 2 to 28 dS m-1) and B (1 to 30 mg l-1) to determine their influence on tree growth, water use, and stable carbon-isotope discrimination. Our results indicate carbon-isotope discrimination (D) was primarily reduced by salinity stress, whereas boron effects were smaller in magnitude and significant only at low salinity. Carbon-isotopic discrimination in leaves of Eucalyptus varied with position in the canopy. For example, proximal leaves sampled low in the canopy D decreased from 23.6 % at low salinity (2 dS m-1 and 1 mg l-1 B) to 22.6 % at high salinity (22 dS m-1 and 1 mg l-1 B). In distal leaves sampled high in the canopy, D decreased from 21.1% to 19.8% in corresponding treatments. Isotopic discrimination in woody tissue from tree trunks also correlated well with salinity stress. Moreover we found the relationship between D and EC of the irrigation water was similar to that of biomass and EC suggesting that D may be useful in describing salt tolerance in as well as quantifying the salt-stress history in C3 trees. There was a significant relationship between isotope discrimination in leaf and wood tissue with transpiration efficiency. The relationship was position sensitive for leaves and correlations with wood tissue increased with time under stress

Proc. 3rd Int. Symp.on Irrigation of Horticultural Crops, Int. Soc. Hort. Sci., Lisbon, Portugal, Jun 28 - Jul 2, 1999.

# STABLE CARBON ISOTOPE DISCRIMINATION: AN INDICATOR OF CUMULATIVE SALINITY AND BORON STRESS IN EUCALYPTUS CAMALDULENSIS

### J.A. Poss, S.R. Grattan, D.L. Suarez and C.M. Grieve

Saplings of *Eucalyptus camaldulensis* Dehn. Clone 4544, irrigated with water of differing salinities (2 to 28 dS m<sup>-1</sup>) and boron concentrations (1 to 30 mg m<sup>-1</sup>), integrated the history of these stresses through the discrimination of stable isotopes of carbon in leaf and woody tissue. Carbon isotope discrimination ( $\Delta$ ) was reduced primarily by salinity. Decreases in discrimination in response to boron stress were detected in the absence of salinity stress, but the decreases were significant only in leaf tissues with visible boron injury. Sapwood core samples indicated that salinity- and boron-induced reductions in  $\Delta$  increased with increasing tree age. Absolute values of  $\Delta$  varied with location of leaf or wood tissue, but relative effects of salinity on the relationship between  $\Delta$  and transpiration efficiency (W) were similar. In response to increasing salinity stress, relative decreases in  $\Delta$  paralleled relative decreases in biomass and both indices yielded similar salt tolerance model parameters. The strong correlations between  $\Delta$ , tree fresh weight, leaf area and W suggest that  $\Delta$  is a useful parameter for evaluating salt tolerance of eucalypts.

Tree Physiol. 20:1121-1127, 2000.

### PISTACHIO ROOTSTOCKS INFLUENCE SCION GROWTH IN PRESENCE OF MIXED SALINITY AND MODERATE BORON

### J.A. Poss, C.M. Grieve, D. Wang, C. Wilson and T.J. Donovan

The salt tolerance of pistachio trees (P. vera) grafted on three rootstocks of pistachio (Pistacia integerrima, P. atlantica, and a P. atlantica x P. integerrima hybrid (UCB-1) was evaluated. Three trees were planted in each of 24 outdoor sand-tank lysimeters and irrigated with saline water containing 10 mg L-1 B. Four salinity treatments (3.5, 8.7, 12 and 16 dS/m in soil water) replicated six times were imposed for six months. Results were evaluated based on shoot biomass, canopy height, number of leaves, leaf area, injured leaf area, trunk diameter, transpiration, stomatal conductance, and SPAD value. The salt tolerance ranking was the same regardless of the growth parameter increase relative to the control trunk resulted in a salt tolerance ranking of P. atlantica (15.2 dS/m) = UCB-1 (16.3 dS/m) > P. atlantica (12.9 dS/m). Reduced SPAD meter values related to lower concentrations of chlorophyll for P. atlantica were associated with a greater degree offoliar injury with this rootstock.

Agronomy Abstract p. 116, 2000.

# TOLERANCE OF HYBRID POPLAR (*POPULUS*) TREES IRRIGATED WITH VARIED LEVELS OF SALT, SELENIUM, AND BORON

### M.C. Shannon, G.S. Bañuelos, J.H. Draper, H. Ajwa, J. Jordahl and L. Licht

Agricultural drainage waters and industrial effluents often consist of waste waters laden with salts, boron (B), selenium (Se), molybdenum (Mo), and other contaminants. However, increasing shortages of high-quality water in arid and semiarid regions and increasing demands to maintain the water quality in rivers, lakes, streams, and groundwater have made water reuse an imperative. Trees have been viewed as potential candidates for wastewater reuse because of their capacities for high evapotranspiration, high growth rates, and abilities to accumulate salts and specific ions in a marketable product that is not biologically hazardous. Clones of eight hybrid poplar (*Populus* spp.) crosses were tested for salt tolerance and ion uptake characteristics in a sand culture study in Riverside, CA. After hardwood cuttings were planted and established under nonsaline conditions, young saplings were treated with artificial waste waters containing different levels of salts, Se, and B. High salt concentrations reduced growth and led to leaf damage and shedding; however, Se and B had no detrimental effect on growth. Salinity affected Se and B accumulation patterns in leaves. A significant degree of genetic variation in salt tolerance was noted among the clones. The salinity at which dry weight was reduced ranged from about 3.3 to about 7.6 dS m<sup>-1</sup> depending on clone, and the relative decrease in dry weight yield with increasing salinity varied among clones and ranged from about 10 to 15% per dS m<sup>-1</sup>. This would indicate that poplars, whereas certainly more salt tolerant than avocado trees, are significantly less salt tolerant than eucalyptus. Leaf Cl concentrations increased in relation to the Cl concentrations in the irrigation waters, but also were subject to clonal variation. Salt tolerance in poplar was generally related to Cl in the leaves and stems but was also influenced by growth and vigor characteristics, as well as the allometric relationships between leaves and stems that influenced the sinks in which ions could accumulate before reaching toxic levels.

Int. J. Phytoremediation 1:273-288, 1999.

# PHYTOEXTRACTION AND ACCUMULATION OF BORON AND SELENIUM BY POPLAR (*POPULUS*) HYBRID CLONES

### G.S. Bañuelos, M.C. Shannon, H. Ajwa, J.H. Draper, J. Jordahl and L. Licht

There as been much interest recently in central California for reusing drainage water to grow trees. A sand-culture study was conducted to investigate the accumulation of boron (B) and selenium (Se) in eight hybrid poplar (Populus) clones irrigated with synthetic agricultural effluent containing increasing levels of chloride salt, B, and Se. Electrical conductivity (EC) ranged from 1.5 to 15 dS m<sup>-1</sup>, B levels from 1 to 5 mg L<sup>-1</sup>, and Se levels from 100 to 500  $\mu$ g L<sup>-1</sup>. Compared with all tree organs, the leaves accumulated the greatest concentrations of B and Se at the time of harvest. The results show that pooled leaf B concentrations were positively correlated with EC levels (r=0.78, P<0.001) and negatively correlated (r=-0.53, P<0.001) with leaf dry matter for all clones at all tested B levels. Combined leaf and stem Se data show, respectively, a significant decrease (P<0.05 level) in tissue accumulation of Se with increased salinity. Toxicity symptoms (e.g., burning leaf margins, shoot die back) occurred in most clones grown at 12 and 15 dS m<sup>-1</sup> treatments leading to leaf abscission. Based on the data, clone 49177 ( $Populus\ trichocarpa\ x\ P.\ deltoidus$ ) best tolerated the tested parameters among the clones and accumulated the greatest amount of B and Se. The moderate ability of the Populus species to remove and accumulate B and Se from saline effluent is most effective at salinity levels less than 7 dS m<sup>-1</sup>.

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### OPTIONS FOR USING LOW-QUALITY WATER FOR VEGETABLE CROPS

#### M.C. Shannon and C.M. Grieve

At least two factors have led to increased interest in using low-quality, high-salinity water to grow crops. The first is the lack of drainage outlets in many agricultural areas of the world. In order to avoid lowering water quality for downstream users, regulations have evolved that mandate on-farm or regional strategies for reuse and/or disposal of saline drainage water. A second factor is that competition between agricultural and urban users for high-quality water has increased as the population has increased. Thus, agricultural users must rely more on low-quality water resources. Traditionally, growers have shifted from salt-sensitive crops to more tolerant species in order to avoid yield losses associated with high salinity. Usually this involves changing from crops of higher cash value to crops of lower value. Vegetable crops are generally less salt-tolerant and have higher cash value than most field and grain crops. Germplasm and management practices need to be improved to provide the grower with more economical and environmentally acceptable options for drainage water reuse. Some investigators have suggested that low-quality and high-quality waters can be used in successive applications during crop rotations or even within a rotation, if applied during growth stages that are more salt-tolerant or salt-sensitive, respectively. The addition of saline water during fruiting of melon (Cucumis melo L.) and tomato (Lycopersicon esculentum Mill.) has even been found to enhance sugar and soluble solid contents and to improve flavor and market price. Although much research is needed to quantitatively define salt-tolerant and salt-sensitive growth stages for vegetables, the potential high cash value of vegetable crops would go far in offsetting the costs of drainage and water delivery systems necessary to implement water reuse practices. Vegetable crops that may be grown using the cyclic water-use strategies may include both traditional and potentially new species.

HortScience 35:1058-1062, 2000.

# ANALYSIS OF SALT TOLERANCE IN NINE LEAFY VEGETABLE SPECIES IRRIGATED WITH SALINE DRAINAGE WATER

M.C. Shannon, C.M. Grieve, S.M. Lesch and J.H. Draper

Saline agricultural drainage water may be used as a resource to grow high value horticultural crops and reduce the volume of drainage for eventual disposal. To explore reuse options the effects of salinity and timing of application were tested on nine vegetable species grown in 24 sand culture plots in Riverside, California. The leafy winter vegetables that were tested included spinach (Spinach oleracea, L.), greens (Brassica rapa), red giant greens (Brassica juncea), Swiss chard (Beta vulgaris), kale (Brassica oleraceae), pac choi (Brassica rapa), tatsoi (Brassica rapa), radicchio (Cichorium intybus), and endive (Cichorium endivia). All vegetables were planted at the same time and initially irrigated with tap water and nutrients having an electrical conductivity of about 3 dS m<sup>-1</sup>. At three and seven weeks salinity treatments were initiated by adding salts to the irrigation water made to the chemical compositions of drainage waters typically found n the San Joaquin Valley, CA. Electrical conductivities of the six salinity treatments were 3 (control), 7, 11, 15, 19 and 23 dS m<sup>-1</sup>. A randomized complete block design was used (6 salinities x 2 application times x 2 replications) and within each plot a 1.5 m row of the nine vegetables were grown as split plots. A random sample of three plants per species was harvested for fresh and dry weight analyses and a statistical modeling approach was developed to analyze the effects of salinity and application time on each vegetable. Salinity reduced fresh weight yields of all species and salination at three weeks further reduced fresh weights in seven of the nine compared to salination at seven weeks. An analysis of salt tolerance curves, maximum yields, and the point of 50 percent yield reduction (C<sub>50</sub>) was made. Greens produced the highest biomass at 874 g per plant but was the most affected by salination time. Chard and radicchio were not significantly affected by timing of salination and chard was the most salt tolerant overall. Red giant greens, kale, pac choi, greens, and to a lesser extent, tatsoi, could all have potential as winter-grown, leafy vegetables in drainage water reuse systems.

J. Amer. Soc. Hort. Sci. 125:658-664, 2000.

### SINGLE CYCLE SELECTION FOR SALT TOLERANCE IN LESQUERELLA FENDLERI (GRAY) S. WATS

M.C. Shannon, D.A. Dierig, C.M. Grieve and J.H. Draper

In a study conducted in 1997-1998, to determine the salt tolerance of *Lesquerella fendleri* (Gray) S. Wats., it was found that saline irrigation above 21 dS/m electrical conductivity resulted in high plant mortality. Replicate Plots having a combined population of 216 plants yielded only five surviving plants at 24 dS/m and 13 survivors at 21 dS/m. In an effort to determine if *Lesquerella* had heritable characters for salt tolerance, surviving plants were inter-mated under controlled conditions and seed was collected from these plants. The following season, on 28 Oct. 1998, seed of the selected salt tolerant full-sibs, designated line 'C', were direct seeded along with two other lines for comparison in a replicated randomized block salinity trial conducted in 21 outdoor sand tanks. Line 'A' was the original seed planted the previous year, and line 'B' was a check line. After seeding,, the tanks were irrigated daily with complete nutrient solutions. Plant populations were thinned to 24 plants/line/plot on 21 Jan. 1999, and salinity was imposed by stepwise additions of mixed salt salinity composed predominantly of Na, Mg, SO<sub>4</sub>, and Cl ions. Over a period of one week, salinity levels in the tanks were increased to 3, 7, 11, 15, 18, 21, and 24 dS/m, with three replications.

Plants were counted and plant heights were measured weekly. At the time of salinization C-line plants were already significantly taller than B- and A-line plants in all plots, 11.7, 6.62, and 4.09 cm, respectively. Within two weeks after salinization significant treatment differences in both plant height and survival were observed among lines due to salinity stress. Plant survival decreased as a function of time and salinity concentration. The parental line A was most sensitive, C-line most tolerant and B-line intermediate. By 25 Feb. none of the A-line plants survived at the 24 dS/m salinity level. Plants were harvested on 15 Jun. and individual dry weights of plants and seed were recorded. Seed was saved for analysis of oil quality. Leaf samples were taken, dried, ground, and weighed to measure ion content.

Analysis of the final shoot dry weights indicated that salinity and line effects were significant but there was no interaction. Salinity decreased average shoot dry weights in all lines as a function of increasing salinity and ranked mean differences within lines were consistent across all salinity levels from 3 to 18 dS/m. At 7, 15, and 18 dS/m average shoot dry weights of the C-line was significantly greater than the parental A-line. The average mean shoo9t weight of B-line was intermediate but always lower than C-line. Our results showed that across all salinity levels, the C-line had higher average shoot dry weights (25.9 g/plant) than either the B-line (17.4 g/plant) or the A-line (11.2 g/plant). Our results indicate that a single cycle selection of Lesquerella in salinized sand cultures resulted in a C-line that had higher absolute and relative salt tolerance as measured by shoot dry matter production, plant height and plant survival. Selected, surviving, C-line plants in the 18, 21 and 24 dS/m plots were either crossed or selfed to provided future information on the inheritance of the salt tolerance character.

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#### SINGLE CYCLE SELECTION FOR SALT TOLERANCE IN LESQUERELLA

### M.C. Shannon, D.A. Dierig, J.H. Draper and C.M. Grieve

A previous salinity study resulted in high mortality in *Lesquerella fendleri* above 21 dS/m electrical conductivity. Surviving plants were inter-mated to determine if Lesquerella had heritable characters for salt tolerance. Seed of the selected full-sibs, line 'C', were direct seeded with two other check lines in a salinity trial conducted in 21 outdoor sand tanks. Salinity was imposed by stepwise additions of mixed salts in irrigation solutions composed of Na, Mg, SO<sub>4</sub>, and Cl ions to 3, 7, 11, 15, 18, 21, and 24 dS/m, with three replications. Plant survival decreased with time and salinity but seed oil increased. None of the A-line checks survived at 24 dS/m. Average shoot dry weights decreased in all lines with increasing salinity and ranked meant differences within lines were consistent across all salinities to 18 dS/m. At 7, 15, and 18 dS/m average shoot dry weights of the C-line was significantly greater than the A-line. Average shoot weight of the B-line was intermediate. Across all salinity levels, the C-line had higher average shoot dry weight than either B- or A-line, 25.9, 17.4, and 11.2 g/plant, respectively. Thus, a single cycle selection of Lesquerella resulted in a C-line that had higher absolute and relative salt tolerance as measured by shoot dry matter production, plant height, and plant survival.

Agronomy Abstract p. 112, 2000.

# USE OF RECYCLED DRAINAGE WATER ON THREE SALT-TOLERANT, WARM-SEASON GRASSES

### M.C. Shannon, J.D. Oster and T.J. Donovan

Drainage water reuse is an important option for the reduction of drainage water volume. Three warm-season grass species were tested for salt tolerance and water use in sand cultures using simulated saline drainage waters. Bermuda grass (*Cynodon dactylon*), silt grass (*Paspalum vaginatum*) and salt grass (*Distichlis spicata*, var NyPa). Saline irrigations were composed of Ca, Na, Mg, SO<sub>4</sub>, and Cl made to solution electrical conductivities of about 6, 10, 16, 24, and 30 dS/m, with the nonsalinized control at 2 dS/m. In 1997, highest yield of silt grass was better than salt grass and Bermuda grass (2106, 1477, and 1410 g/m² dry weight, respectively. In 1998, salinities were increased to 6, 10, 16, 20, 30, and 45 dS/m. Maximum yields of silt grass (2112 g/m²) were obtained at 10 dS/m. Maximum yield of Bermuda grass (2014/g/m²) and salt grass (1432 g/m²) were obtained at 16 dS/m. Salinity increase ash content and significantly reduced digestible fiber content (ADF and NDF). Increasing salinity generally decreased Ca and K contents of shoots and increased Na and Cl.

Agronomy Abstract p. 179, 2000.

# EMERGENCE AND SEEDLING GROWTH OF SOYBEAN CULTIVARS AND MATURITY GROUPS UNDER SALINITY

### D. Wang and M.C. Shannon

Soybean is an important agricultural crop and has, among its genotypes, a relatively wide variation in salt tolerance. As measured by vegetative growth and yield, however, the achievement or failure of a high emergence ratio and seedling establishment in saline soils can have significant economic implications in areas where soil salinity is a potential problem for soybean. This study was conducted to determine the effects of salinity, variety and maturation rate on soybean emergence and seedling growth. Included in the study were the variety 'Manokin'; four near-isogenic sibling lines of the variety 'Lee' belonging to maturity groups IV, V, VI and VII; and the variety 'Essex' and two of its near-isogenic related lines representing maturity groups V, VI and VII, respectively. Field plots were salinized with sodium chloride and calcium chloride salts prior to planting. The soybeans were irrigated with furrow irrigation which redistributed the salts towards the tail ends of the field plots. Elevated soil salinity near the tail ends of the field significantly reduced soybean emergency rate, shoot height and root length. No significant reduction was found for emergence or seedling growth of variety 'Manokin' when the electrical conductivity of soil solution extract (ECe) was less than 3 dS m<sup>-1</sup>. Soybean emergence and seedling growth was significantly reduced when soil ECe reached about 11 dS m<sup>-1</sup>. Maturity groups V and VII of variety 'Lee' or V and VI of 'Essex' appeared to be more sensitive to salinity stress than other maturity groups. Salt tolerance of different genotypes and maturity groups should be considered, among other limiting factors, in minimizing salinity effects on soybean growth.

Plant and Soil, 214:117-124, 1999.

# SOIL WATER AND TEMPERATURE REGIMES IN DRIP AND SPRINKLER IRRIGATION, AND IMPLICATIONS TO SOYBEAN EMERGENCE

### D. Wang, M.C. Shannon, C.M. Grieve and S.R. Yates

Irrigation has long been used in agriculture as a primary means of water management. It is well known that water distributions in the soil differ depending on the methods of irrigation. However, it is less clear how soil thermal regimes would change over time and space when irrigation methods are different. A field study was conducted to investigate the interactive effect of soil water and temperature regimes in drip and sprinkler irrigation. The effect of different methods of irrigation on soil water and thermal environment was then used to interpret differences in soybean emergence and seedling growth under the two irrigation treatments. Time domain reflectometry wave-guides and thermocouples were installed in field plots to provide soil water content and temperature measurements. Soybean seeds were planted to assess the emergence and seedling development. Consistent with infiltration theory, soil water contents were higher directly under the drip tapes in drip irrigation, but were relatively more uniform across the whole soil surface in sprinkler irrigation. Although five times more water was used in the sprinkler than in the drip plot, the soil water content at the seed zone was similar. Soil temperature was significantly higher in the drip than in the sprinkler plot, which led to a higher emergence rate and enhanced seedling growth. Drip irrigation not only conserved water but also maintained the soil profile at a higher temperature more favorable for plant emergence and seedling development.

Agric. Water Management 43:15-28, 2000.

# SOYBEAN CANOPY REFLECTANCE UNDER DIFFERENT SALINITY AND IRRIGATION TREATMENTS

### D. Wang, C. Wilson and M.C. Shannon

High levels of soil and water salinity can strongly decrease plant growth rate, reducing yield and quality in agricultural and horticultural crops. Effects of salinity may be determined by measuring reflectance characteristics of plant canopies before final yield reduction occurs. Spectral reflectance of the soybean canopy was measured over time using a hand-held multispectral radiometer. To relate the reflectance with salinity and irrigation effects, leaf chlorophyll contents were determined from chlorophyll concentrations measured with a Minolta SPAD-502 meter and leaf areas measured from destructive plant samples. For soybeans grown under salinity, canopy reflectance in the 810 to 950 nm or NIR spectrum region was about 10% lower than plants not treated with salinity, regardless of the irrigation method employed. The reflectance decrease in NIR and a small increase in the red spectrum region resulted in reductions in calculated normalized difference vegetation index or NDVI. The reflectance increase in the red spectrum region was due to losses of chlorophyll from salinity stress. The critical time to detect salinity effects by reflectance measurements was near the end of plant vegetative growth phase before maturation and senescence had begun.

Agronomy Abstract p. 16, 1999.

## SALINITY DISTRIBUTION UNDER DRIP AND SPRINKLER IRRIGATION AND EFFECTS ON SOYBEAN GROWTH

### D. Wang, M.C. Shannon, T.J. Donovan and C.M. Grieve

Crop salt tolerance research traditionally reports crop yield response on the basis of average root-zone soil salinity. Soil salinity, however, is seldom uniform; the spatial and temporal distributions of soil salinity under field conditions are highly dynamic, and are functions of irrigation and plant water extraction. This study was conducted to determine the characteristics of salinity distribution under different irrigation regimes and to correlate these distributions with soybean growth parameters. Salinity effects were imposed by irrigation with salinized water (NaCl and CaCl<sub>2</sub>, 1:1 by weight). Detailed soil salinity and water content measurements were obtained with time-domain reflectometry over time and space. Measured soybean growth parameters were plant height, root length, biomass accumulation of plant shoot and root, and leaf area. Results indicated that the spatial and temporal distributions of soil salinity were different depending on the methods, amount, and salinity levels of the irrigation. More salt accumulation was found in the soil profile in the drip than in the sprinkler irrigation plot. Drip irrigation created a region of high soil salinity in the 20 to 30 cm depth range which limited root penetration. Salinity and irrigation treatment resulted in water stress and reduced soybean shoot development.

Agronomy Abstract p. 283, 1999.

## SOIL WATER AND TEMPERATURE REGIMES IN A SAND CULTURE FOR SCREENING PLANT SALT TOLERANCE

#### D. Wang, T.J. Donovan and M.C. Shannon

Because of the high spatial and temporal variability in soil salinity under field conditions, plant salt tolerance studies are often conducted in greenhouse sand cultures for better salinity control. This study was conducted to determine soil water and temperature regimes in the sand cultures and to compare with a field soil. Results indicated that sand cultures with well-graded texture, such as the washed river sand, can provide water and thermal regimes comparable to a field soil. If other environmental factors for the plant growth can be simulated to match that in field conditions, results of plant salt tolerance obtained from the sand cultures can be used to provide guidance for plant selection under field conditions. A more realistic approach for salt tolerance studies in the sand cultures is to create a set of sand media with gradual salinity changes over time and space simulating soils of different textures such as loamy sand, silt loam, or clay.

Agronomy Abstract p. 201, 2000.

# GROWTH STAGE MODULATES SALINITY TOLERANCE OF NEW ZEALAND SPINACH (Tetragonia tetragonioides, pALL.) AND RED ORACH (Atriplex hortensis L.)

C. Wilson, S.M. Lesch and C.M. Grieve

The response of two speciality vegetable crops, New Zealand spinach (Tetragonia tetragonioides Pall.) and red orach (Atriplex hortensis L.), to salt application at three growth stages was investigated. Plants were grown with a base nutrient solution in outdoor sand cultures and salinized at 13 (early), 25 (mid), and 42 (late) d after planting (DAP). For the treatment salt concentrations, we used a salinity composition that would occur in a typical soil in the San Joaquin Valley of California using drainage waters for irrigation. Salinity treatments measuring electrical conductivities (EC<sub>1</sub>) of 3, 7, 11, 15, 19 and 23 dS m<sup>-1</sup> were achieved by adding MgSO<sub>4</sub>, Na<sub>2</sub>SO<sub>4</sub>, NaCl and CaCl<sub>2</sub> to the base nutrient solution. These salts were added to the base nutrient solution incrementally over a 5-d period to avoid osmotic shock to the seedlings. The base nutrient solution without added salts served as the non-saline control (3 dS m<sup>-1</sup>). Solution pH was uncontrolled and ranged from 7.7 to 8.0. Both species were salt sensitive at the early seedling stage and became more salt tolerant as time to salinization increased. For New Zealand spinach, the salinity levels that gave maximal yields (C<sub>max</sub>) were 0, 0 and 3•1 dS m<sup>-1</sup> and those resulting in a 50% reduction of biomass production (C<sub>50</sub>) were 9•1, 11•1 and 17•4 dS m<sup>-1</sup> for early, mid and late salinization dates, respectively. Maximal yield of red orach increased from 4•2 to 10•9 to 13•7 dS m<sup>-1</sup> as the time of salinization increased from 13, to 26, to 42 DAP, respectively. The C<sub>50</sub> value for red orach was unaffected by time of salt imposition (25 dS m<sup>-1</sup>). Both species exhibited high Na<sup>+</sup> accumulation even at low salinity levels. Examination of K-Na selectivity data indicated that K<sup>+</sup> selectivity increased in both species with increasing salinity. However, increased K-Na selectivity did not explain the increased salt tolerance observed by later salinization. Higher Na-Ca selectivity was determined at 3 dS m<sup>-1</sup> in New Zealand spinach plants treated with early- and mid-salinization plants relative to those exposed to late salinization. This corresponded with lower  $C_{max}$  and  $C_{50}$  values for those plants. Lower Ca uptake selectivity or lower Ca levels may have inhibited growth in young seedlings. This conclusion is supported by similar results with red orach. High Na-Ca selectivity found only in the early-salinization plants of red orach corresponded to the lower  $C_{max}$  values measured for those plants.

Annals of Bot. 85:501-509, 2000.

# EFFECT OF SULFATE-BASED SALINITY ON GROWTH OF BARNYARDGRASS (Echinochola crus-galli L. Beauv.)

#### C. Wilson and J.J. Read

High-quality water needed for agriculture is becoming increasingly scarce due to changing environmental standards and rising demands from urban areas. Several irrigation schemes have been proposed to utilize higher salinity waters. However, growth under saline conditions could alter the competition between weeds and crops. Information on the effects of saline irrigation waters on weed growth is limited. In this study, we investigated the effect of sulfate-based salinity on the growth responses of a C4-weed, barnyardgrass. Barnyardgrass was harvested following 41 days of sanitization when most plants were at the jointing or booting stage of development. Previous reports on growth responses of crop plants to salinity were interpreted in terms of a linear two-piece model. Across the four salinity treatments, 3 (control), 7, 11, and 19 dS m-1, our data on barnyardgrass were better described by a quadratic function. Data were analyzed using analysis of variance and general linear models in SAS. Values for fresh weigh per plant on dS m-1 indicated a highly significant (P<0.002) linear relationship. Fresh weight decreased significantly (F ratio = 6.53; P<0.003) as salinity increased, and was least at 19 dS m-1. The linear salt tolerance model had a slope of -0.08 (SE = 0.02) and a C50 value of about 14.3 dS m-1. Total-S, total-P, Ca<sup>+2</sup>, Mg<sup>+2</sup>, Na<sup>+</sup>, and K<sup>+</sup> in shoots were measured. The role of these ions in salinity tolerance will be discussed.

Weed Science Society of America Abstracts p. 49, 1999.

### EFFECT OF EXOGENOUS POLYAMINES ON SPINACH GROWTH AND CARBOHYDRATE METABOLISM

#### C. Wilson, S. Suleiman and L. Zeng

Salt-induced suppression of crop yield is a major problem in irrigated areas. Polyamines, a new class of growth regulators, are thought to be involved in plant responses to stress. We investigated the effect of the exogenously supplied polyamines, putrescine, spermine, and spermadine, on spinach (*Spinacia oleracea* L, cv. Space) growth. In order to investigate the effect of salinity on growth mechanism(s), we examined photosynthesis and sugar (glucose, fructose, and sucrose) levels. Salinity significantly affected growth with decreased growth measured at the higher salinity levels. However, we did not observe any significant changes in photosynthesis with increasing salinity. Exogenously supplied polyamines had no measurable effect on salt-induced growth suppression. Increasing salinity did alter the diurnal pattern of sugar levels. While salinity decreased afternoon levels of glucose, it had no effect on morning levels. Conversely, morning levels of sucrose increased with increasing salinity while afternoon levels were not affected. We found no effect of salinity on fructose levels, regardless of time of day. Polyamines application did not affect this pattern. The relationship between salinity and diurnal carbohydrate metabolism will be discussed.

Agronomy Abstract p. 97, 1999.

### SALINITY EFFECTS ON SEEDLING GROWTH AND YIELD COMPONENTS OF RICE

#### L. Zeng and M.C. Shannon

Flood irrigation practices that are commonly used in California during the early stages of rice (Oryza sativa L.) establishment may contribute to salinity damage and eventually decrease yield. Knowledge of salinity effects on rice seedling growth and yield components would improve management practices in fields and increase our understanding of salt tolerance mechanisms in rice. Salinity sensitivity of rice was studied to determine salinity effects on seedlings and yield components. Plants of rice cultivar M-202 were grown in a greenhouse in sand and irrigated with nutrient solutions of control and treatments amended with NaCl and CaCl<sub>2</sub> (2:1 molar concentration) at 1.9, 3.4, 4.5, 6.1, 7.9, and 11.5 dS m<sup>-1</sup> electrical conductivity. Shoot dry weights of seedlings were measured at five harvests in the first month after seeding. Seedling growth was significantly reduced by salinity at the lowest salinity treatment, 1.9 dS m<sup>-1</sup>. At 1.9 and 3.4 dS m<sup>-1</sup>, significant reduction of seedling growth occurred at longer cumulative thermal time than at higher salt levels. Seedling survival was significantly reduced when salinity 3.40 dS m<sup>-1</sup> and higher. Highly significant linear responses of grain weight per plant, grain weight per panicle, spikelet number per panicle, and tiller number per plant to salinity were observed. There was a common lowest salt level for fertility and pollen germination beyond which they were significantly reduced by salinity. Harvest index was significantly decreased when salinity was at 3.40 dS m<sup>-1</sup> and higher. Tiller number per plant and spikelet number per panicle contributed the most variation in grain weight per plant under salinity. Reductions in seedling survival, tiller number per plant, and spikelet number per panicle were the major causes of yield loss in M-202 under salinity. The compensation between spikelets and other yield components was confounded with salinity effects, but was believed to be minor relative to the reduction of spikelets due to salinity and, therefore, not sufficient to offset yield loss even at moderate salt levels.

Crop Sci. 40:996-1003, 2000.

### EFFECTS OF SALINITY ON GRAIN YIELD AND YIELD COMPONENTS OF RICE AT DIFFERENT SEEDING DENSITIES

#### L. Zeng and M.C. Shannon

Substantial loss of plant stand and yield reduction have been observed in salt-affected, direct water-seeded rice (Oryza sativa L.). One of the possible management options for growers in dealing with decreases in rice production caused by salinity is to compensate yield reduction due to loss of plant stand during early stages by increasing seeding density. The objectives of this study were to investigate the effects of salinity and seeding density on grain yield and yield components, and analyze the relationships of the yield components to final grain yields at different seeding densities under salinity. Plants were grown in the greenhouse in silica sand irrigated with nutrient solutions. The treatments included seeding densities of 400, 600 and 720 seeds m<sup>-2</sup> and salt levels of 1.0, 3.9 and 6.5 dS m<sup>-1</sup>. Yield components were measured on individual plants and grain yields were measured on an unit area basis. Salinity effects were highly significant on grain yield, plant stand, seed weight per plant, seed weight per panicle and spikelets per panicle at each seeding density, but not significant on panicle density and kernel weight. Grain yield was not significantly increased with an increase of seeding density. Plant stand and panicle density were significantly increased while seed weight per plant and fertility were significantly decreased with increases of seeding densities. Seed weight per panicle accounted for 63% of total variation and contributed more than panicle density to the grain yield under salinity. It was concluded that yield loss under moderate salinities may not be compensated by increasing seeding density above normal density levels. Other management options or new cultivars with improved salt-tolerance must be developed.

Agronomy J. 92:418-423, 2000.

### TIMING OF SALINITY STRESS AFFECTS RICE GROWTH AND YIELD COMPONENTS

#### L. Zeng, M.C. Shannon and S.M. Lesch

The irrigation schemes in rice production have accelerated soil salinization processes and raised salt levels in standing water of rice fields in many regions. Substantial loss in plant stand and final yield reduction were observed in some salt-affected rice fields in California. Salinity problems in salt-affected rice fields might be relieved by developing appropriate management options for rice growers. Our previous studies have shown that increasing seeding density was not an effective method to ameliorate rice yield reduction under salinity. The development of other management options requires the analysis of sensitivity parameters which affect the interaction between salinity and crop yield. Timing of salinity stress is one such parameter which has rarely been reported. Plants were grown in silica sand irrigated with nutrient solutions in a greenhouse. Plants were salinized and stress was relieved at different growth stages. Plant shoot dry weight was analyzed at both seedling and mature stages. Yield components were analyzed at final harvest. The effects of salinity and timing were significant on plant growth and most yield components. Panicle initiation was identified as the most salt-sensitive stage affecting grain yield. The relationship between vegetative growth and final grain yield was also analyzed.

Agronomy Abstract p. 97, 1999.

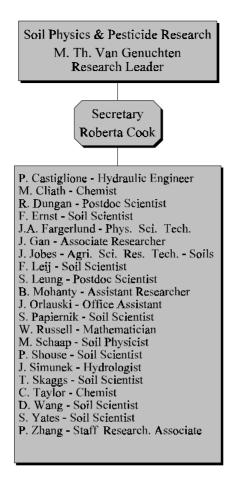
### EVALUATION OF SALT TOLERANCE IN RICE GENOTYPES BY MULTIPLE PARAMETERS

#### L. Zeng, M.C. Shannon, C.M. Grieve and J.A. Poss

This study was designed to identify the agronomic parameters contributing to salt tolerance in seed yield and evaluate genotypes of different sources on multiple parameters for salt tolerance. Plants were grown in a greenhouse in sand and irrigated with nutrient solutions of control and treatments amended with NaCl and CaCl<sub>2</sub>. Wide genotypic differences in relative salt tolerance of seedling growth were identified among genotypes. Reproductive growth including panicle initiation and anthesis was delayed in all genotypes. Spikelet number per panicle, tiller number per plant, and seed weight per panicle were significantly reduced by salinity in most genotypes. Wide genotypic differences in relative salt tolerance of these yield components were identified among genotypes. No genotypic difference was identified for fertility and kernel wight among genotypes. The means of the salt tolerance indexes in the multiple parameters were analyzed simultaneously using a multivariate analysis. The genotypes were ranked for salt tolerance at different growth stages based on multivariate analysis. Spikelet number per panicle and tiller number per plant were suggested as a multiple selection criteria in the screening for salt tolerance.

Agronomy Abstract p.191, 2000

# Soil Physics & Pesticide Research



#### Mission

The mission of the Soil Physics & Pesticide Research unit is to develop methods for evaluating, predicting, and managing the movement of water, salts and agricultural chemicals in the root and vadose zones of salt-affected soils, and to develop tools for assessing new soil-water-crop management schemes to make effective use of limited resources where salinity and/or pesticides area concern. Emphasis is on (1) evaluating the impact of irrigated agriculture on soil and groundwater quality using integrated unsaturated water and solute transport models related user-friendly computer software, (2) pesticide volatilization and pesticide loadings from agricultural fields to surface and ground waters, (3) developing improved methods for measuring unsaturated water and solute transport parameters and related soil properties, (4) characterizing the important physical and chemical processes affecting the fate and transport of harmful pesticides and related organic chemicals into the atmosphere and into the subsurface, and (5) developing methods for evaluating and reducing soil and water contamination by pathogens from the use of animal waste products.

#### SOIL PHYSICS & PESTICIDE RESEARCH STAFF



#### MARTINUS Th. van GENUCHTEN, B.S., M.S., Ph.D., Research Leader and Supervisory Soil Scientist of the Soil Physics & Pesticide Research.

Water flow and solute transport in soil and groundwater systems. Analytical and numerical methods for simulating water, heat and/or solute movement in the subsurface. Characterization and measurement of the unsaturated soil hydraulic properties. Use of inverse methods for estimating vadose zone flow and transport parameters. Crop salt tolerance. Root water uptake. Reclamation of salt-affected soils. Preferential flow of water and solutes in

aggregated (macroporous) soils and fractured rock. Pesticide transport. Nonequilibrium chemical transport.

## SCOTT R. YATES, B.S., M.S., Ph.D. Soil Scientist for Soil Physics & Pesticide Research

Pesticide fate and transport as related to the quality of surface and groundwaters in irrigated areas; test and develop analytical and numerical solutions for the transport of organic compounds in heterogeneous porous media, especially at field scale. Application of models for simulating saturated and unsaturated flow, solute, heat and vapor transport in the subsurface, including the effects of surface volatilization. Other areas of interest include microbial transport, hillside seepage processes, applications of geostatistics and other techniques for describing field-scale spatial variability.





# SHARON PAPIERNIK, B.A., Ph.D., Soil Scientist for Soil Physics & Pesticide Research.

Laboratory and field investigations of the environmental fate of pesticides; sorption/desorption, transformation, and transport of fumigants and other pesticides and the interaction of these processes; development of management practices to minimize environmental contamination by pesticides while maintaining efficacy; improved methods of laboratory analysis of pesticides and their properties.

#### SOIL PHYSICS & PESTICIDE RESEARCH STAFF



DONG WANG, B.S., M.S., Ph.D., E.I.T. Soil Scientist for Soil Physics & Pesticide Research.

Drip, sprinkler, furrow irrigation systems; processes and mechanisms attributing to soil and water salinity; environmental biophysical factors affecting plant growth under saline environment; heat and mass transfer in the soil-water-plant-atmosphere continuum.

# TODD SKAGGS, B.S., Ph.D., Soil Scientist for Soil Physics & Pesticide Research.

Field, laboratory, and theoretical investigations of flow and transport processes in soils; fate and transport of salts and agricultural chemicals in groundwater; improved methods for treating spatial and temporal variability.





PETER J. SHOUSE, B.S., Ph.D., Soil Scientist for Soil Physics & Pesticide Research.

Laboratory and field investigations that quantify the fundamental processes of water and salt movement in naturally heterogeneous soils, and the response of plants to water and salinity stress.

### MULTI-FLUID HYDRAULIC PROPERTIES FOR FRACTIONAL WETTABILITY POROUS MEDIA

#### S.A. Bradford, L.M. Abriola and F.J. Leij

The theory for the prediction and modeling of multiphase hydraulic properties has largely relied on the simplifying assumptions that water completely wets the solid surface and, in the case of three-fluid systems, that the organic spreads to form a continuous intermediate wetting phase. More complex fluid distributions may occur in many natural systems due to spatial and temporal variations in fluid and solid properties. In some instances the porous media can have both water- and organic-wet solid surfaces. This condition is referred to as fractional wettability. This paper reviews methods that have been developed by the authors over the past several years to measure, model, and predict hydraulic property relations for fractional wettability soils containing two (organic liquid and water) or three (air, organic liquid, and water) fluids. Fractional wettability systems exhibited saturation dependent wettability effects on the hydraulic property relations. For a given saturation history, increasing the organic-wet fraction tended to decrease the organic relative permeability and the organic-water capillary pressure (organic minus water pressure). The predictive procedures discussed herein were assessed with independent experimental data. Results indicate that these methods, used in conjunction with wettability indices, could provide reasonable predictions of the fractional wettability hydraulic properties. The predictions for three-fluid systems were more speculative due to the formation of a discontinuous intermediate phase, and the lack of relative permeability data for model comparison.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 165-178, University of California, Riverside, CA, 1999.

### MEASUREMENT OF INITIAL SOIL-WATER CONTACT ANGLE OF WATER REPELLENT SOILS

#### M.L.K. Carrillo, J. Letey and S.R. Yates

Water repellent soils are common throughout the world. Water repellency significantly affects infiltration, evaporation, and other water-soil interactions. Various indices, such as the water-solid contact angle ( $\theta$ ), water drop penetration time (WDPT), and 90° surface tension ( $\gamma_{ND}$ ), have been proposed to characterize the degree of water repellency. The water repellency of many soils is not stable, but changes with time after contact with water. No method is available to measure the initial soil-water contact angle. The purpose of this study was to establish a technique to measure the initial soil-water contact angle. We combined previously published theoretical relationships to develop the equations  $\cos \theta = [(\gamma_{ND}/\gamma_{W})^{1/2} - 1]$  and  $h_p = 2[(\gamma_w \gamma_{ND})^{1/2} - \gamma_w]/r\rho g$ , where  $\gamma_w$  is the water surface tension,  $h_p$  is the breakthrough pressure head, r is the pore radius,  $\rho$  is the water density, and g is the gravitational constant. The validity of these relationships was established by treating two sand materials with octadecylamine or solvent extracts from peat moss to create various levels of water repellency. An instrument was developed to measure  $h_v$ . A linear relationship was found between  $h_p$  and  $\gamma_{ND}^{1/2}$  as specified by the equation. The value of r was computed from the slope  $h_p vs.$   $\gamma_{ND}^{1/2}$  curve, and this r value was combined with  $h_p$  in the capillary rise equation to compute  $\cos \theta$ . Good agreement was found between measured and predicted relationships between  $\cos\theta$  and  $\gamma_{ND}$  1/2. The major conclusion is that the value of  $\theta$  can be determined by measuring  $\gamma_{ND}$ , which is easily done in the field or laboratory.

Soil Sci. Soc. Am. J. 63:433-436, 1999.

### UNSTABLE WATER FLOW IN A LAYERED SOIL: I. EFFECTS OF A STABLE WATER-REPELLENT LAYER

#### M.L.K. Carrillo, J. Letey and S.R. Yates

The development of preferential water flow in a soil profile can cause accelerated movement of pollutants to the groundwater thus reducing groundwater quality. This study investigated the effects of a stable water-repellent soil layer on the development of unstable water flow in a homogenous profile. Stable w~ter-repellent soil is defined as one whose degree of water repellency does not change with time after contact with water. The effects of water entry pressure  $(h_p)$ , water-repellent layer depth (L) and depth of ponded water at the soil surface  $(h_0)$  on the development of unstable flow were investigated using homogenous coarse sand packed into a specially built rectangular chamber. The hydraulic conductivity of the water repellent soil was also measured as a function of  $h_p$  and  $h_0$  in a separate experiment using the constant head method. The hydraulic conductivity and the water content of the water repellent soil increased as  $h_0/h_p$  increased. No water penetrated the water repellent layer for values of  $(h_0 + L)/h_p < 1$ , unstable flow developed for values between 1 and 1.5 and a stable front developed for values > 1.5. The conclusion is that stable flow occurred when the water flux through the water repellent layer exceeded the saturated hydraulic conductivity of the underlying wettable layer. The water flux through the water repellent layer was a function of the hydraulic conductivity of the water repellent layer which increased as  $h_0/h_p$  increased.

Soil Sci. Soc. Am. J. 64:450-455, 2000.

### UNSTABLE WATER FLOW IN A LAYERED SOIL: II. EFFECTS OF AN UNSTABLE WATER-REPELLENT LAYER

#### M.L.K. Carrillo, J. Letey and S.R. Yates

Water repellent soils are found throughout the world and can exhibit significantly different water flow characteristics as compared to a wettable soil. The purpose of the study was to determine the significance of the stability of the water repellency on the development of unstable water flow below a water repellent layer. Unstable water-repellent soil refers to a soil whose degree of repellency changes with time after contact with water. Experiments were conducted in a specially built rectangular chamber where wetting front patterns could be observed through a Plexiglas sheet. The experiments were done on water repellent sand layers that were treated to create water drop penetration time (WDPT) values of 1, 10, and 150 min. The WDPT of the layer and the ratio  $(h_0 + L)/h_0$  were important in the development of ringers, where  $h_0$  is the depth of ponded water at the soil surface, L is the depth of the water repellent layer and  $h_0$ is the water entry pressure head of the water repellent layer. For low WDPT (1 min) no fingers formed. As the WDPT increased, the tendency for finger formation also increased. The medium WDPT (10 min) layer caused finger formation, however, the fingers broadened and converged after continued flow and an almost uniform wetting front eventually developed. The combination of a high WDPT (150 min) and  $(h_0 + L)/h_0$ <1 produced the most dramatic and persistent fingering. The finger development across the layer and the flux through the layer was found to be a function of time. Water repellency at the soil surface has the greatest impact on infiltration because water depth may not be sufficient to overcome the water entry pressure and runoff would decrease the time of exposure to water to overcome unstable water repellency.

Soil Sci. Soc. Am. J. 64:456-459, 2000.

#### MEASUREMENT OF SOLUTE RESIDENCE CONCENTRATION IN VARIABLY-SATURATED SOILS BY TIME DOMAIN REFLECTOMETRY: A NEW CALIBRATION PROCEDURE

#### P. Castiglione, B.P. Mohanty, P.J. Shouse and M. Th. van Genuchten

Traditionally the TDR technique for measuring solute residence concentration is based on measurement of the d.c. electrical conductivity of bulk soil, which is strongly dependent on the water content and its solute concentration. A pulse voltage propagating through the transmission line, made up of the TDR probe - soil system, is subject to dispersion and attenuation, depending on the dielectric permettivity and electrical conductivity of the soil. Since no exact model for the wave propagation in TDR-soil systems is available, the above characteristics are usually deducted from the analysis of the reflected signal in the time domain, through calibration procedures.

The simplified lumped-circuit model of Giese Tiernann is commonly employed to relate the d. c. conductivity of the soil to the attenuation of the reflected signal at large time, which correspond to low frequencies as stated by the Fourier theory. We carried out a series of measurements in electrolytic solutions for different probe and coaxial cable lengths. Our results showed that this kind of analysis is inadequate if the losses along the cable are not adequately taken into account. A discussion of a distributed-circuit model proposed by Dalton and van Genuchten (1986) is also reported.

The relationship among bulk soil electrical conductivity, water content and solute residence concentration is a characteristic of the soil, and depends on its pore size distribution. Therefore, it can only be determined by a calibration procedure. Usually this consists of TDR measurement of the electrical conductivity in several samples at equilibrium. The water content and solute resident concentration of the samples are then independently measured.

We propose a new calibration procedure, which is based on a series of drainage-leaching cycles on a single soil column. Our procedure utilizes the advantage of measuring the electrical conductivity and the water content over the same sample volume by using the TDR technique. Our experimental results show that within a range of water contents, whose range depends on the soil type, it is possible, by means of the dimensional analysis, to determine a unique relationship among the above mentioned quantities. This procedure, moreover, allows one to easily take into account the electrical conductivity of the solid matrix of the soil, which is often non-negligible.

### QUANTIFICATION OF SOIL MACROPORE/MATRIX PROPERTIES USING CONTRIVED COLUMN EXPERIMENTS

#### P. Castiglione, B.P. Mohanty, P.J. Shouse and M. Th. van Genuchten

Preferential flow is recognized to occur in many agricultural soils. This process is defined as the rapid movement of water and solutes via larger pores bypassing the micropores. Multi-domain models account for the non-equilibrium phenomena characterizing flow/transport in such a condition. Yet, inability to determine the hydraulic/transport properties of each domain separately, severely limits their use. The main goal of this research is to study hydraulic characteristics of the matrix and macropore domains and to investigate the conditions needed for the preferential flow to be activated. A repacked soil column with artificial macropores was designed and created. In this paper, results of transient and steady state infiltration experiments with a non-reactive tracer are presented. The influence of pore geometry as well as the initial and boundary conditions on the macroscopic features of the flow-transport phenomena is discussed.

Agronomy Abstract p. 194, 1999.

### FLOW AND TRANSPORT THROUGH A BIPOROUS MEDIUM: EXPERIMENTAL FINDINGS AND NUMERICAL MODELING

#### P. Castiglione, B.P. Mohanty, P.J. Shouse and M. Th. van Genuchten

Prior research findings show that flow and transport through macroporous medium need to be characterized by nonequilibrium. processes between high and low permeability domains. Such phenomena are usually modeled at the Darcy scale by adopting a multi-domain model based on up-scaling of microscopic heterogeneity to macroscopic processes. In this paper we present flow and transport experimental results from a soil column containing artificial macropores of known geometry. Multiple TDRs located at different depths of the column allowed the monitoring of water and solute breakthrough curves (BTCs) at these depths. Different forward and inverse models were used to analyze BTC data at single or multiple depths. Our analysis revealed inadequacy of such methods using a single BTC. We also showed limitations of the widely adopted Mobile-Immobile model when the soil matrix conductivity is significant with respect to macropore conductivity. Our findings suggest that the macroscopic features of the preferential flow process are strongly dependent on the observation scale. Based on our controlled experimental data we proposed a new physically based procedure for the estimation of transport parameters of a dual-permeability model.

Agronomy Abstract p. 217, 2000.

### ON-LINE SYSTEM FOR VOLATILIZATION MEASUREMENT OF VOCS FROM SOIL

F.F. Ernst, J. Gan, C. Taylor, Q. Zhang, S.K. Papiernik and S.R. Yates

Volatilization of organic compounds is traditionally measured by first trapping the organic vapors on an adsorbent and then quantifying the concentration following sample preparation. This approach is expensive, labor intensive and time consuming, which generally prohibits extensive sample collection. We developed an on-line sampling system that performs real-time sample collection and analysis. Vapors leaving the soil surface are directly swept into a GC, while the use of computer-controlled multiple channels and solenoid valves allows automatic and sequential measurement from multiple volatilization sources. No adsorbent or solvent is needed, and manual input is minimal. This technique was used for continuously measuring emission of three soil fumigants from four soil columns for 11 days, and was found to generate extremely detailed and descriptive volatilization dynamics for each fumigant from each column.

Agronomy Abstract p. 184, 1999.

### APPLICATION OF AMMONIUM THIOSULFATE TO REDUCE TELONE II EMISSIONS FROM SOIL

#### J. Gan, S.K. Papiernik, J.O. Becker, J.A. Knuteson and S.R. Yates

The anticipated phase-out of methyl bromide (MeBr) has stimulated an intensive search for effective alternatives. 1,3-Dichloropropene (Telone II, or 1,3-D), used alone or in combination with chloropicrin, is considered as one of the most promising MeBr replacements. However, both isomers of 1,3-D are highly volatile. A number of studies have shown that 11-90% of applied 1,3-D can escape into the air after soil fumigation. Because 1,3-D is acutely toxic and potentially carcinogenic, excessive emissions of its vapor into the atmosphere may contribute to air pollution and cause detrimental effects to human health and the environment. Thus, in order to continue Telone fumigation in an environment-compatible manner, it is important to develop mitigation practices to reduce its emissions while sustaining its effectiveness for pest control.

Atmospheric emissions of a fumigant can be reduced if the fumigant's volatility is eliminated because of degradation or transformation of the parent compound. In our recent work we have identified thiosulfate products as highly efficient reactants for MeBr, 1,3-D, chloropicrin, methyl iodide, and propargyl bromide. Thus, thiosulfate products may be used as surface reactants to suppress emissions of these fumigants. As ammonium and potassium thiosulfates are commercial fertilizers, this mitigation approach is cost-effective and simple to implement. Here we report transformation of 1,3-D by ammonium thiosulfate (ATS) in soil under different conditions, and experiments demonstrating reduction in Telone II emissions after surface amendment of ATS.

Transformation of 1,3-D in ATS-amended soil was proportional to the relative ratio of ATS to 1,3-D. As shown in Table 1, the half-life of 1,3-D in soil was reduced from 256 h (-10 d) in the non-amended soil to 18 h when the ratio was 2: 1, and further to only 4 h when the ratio was 4: 1. Similar relationships between ATS amendment levels and 1,3-D transformation were observed for both Arlington and Carsitas soils, indicating that ATS-induced 1,3-D transformation was independent of soil type (Table 1). Overall, as the ratio of ATS to 1,3-D was doubled, the half-life of 1,3-D was halved.

We subsequently conducted column experiments to evaluate the reduction of 1,3-D emissions by surface amendment of ATS. In large columns packed with Arlington sandy loam, 1,3-D emission rate (% of applied dosage) decreased rapidly with increasing ATS application rate (Figure I). When ATS was applied in 9 mm water at 64 g  $\,\mathrm{m}^2$ , total 1,3-D emission was reduced by 61%. The reduction increased further to 89% when ATS was applied at 193 g  $\,\mathrm{m}^2$ .

Proceedings of the 1999 Annual International Research Conference on Methyl Bromide Alternatives and Emissions Reductions. Nov. 1-4, 1999, San Diego, CA. 94:1-3, 1999.

### EVALUATION OF ACCELERATED SOLVENT EXTRACTION (ASE) FOR ANALYSIS OF PESTICIDE RESIDUES IN SOIL

#### J. Gan, S.K. Papiernik, W.C. Koskinen and S.R. Yates

Accelerated solvent extraction, or ASE, is a new extraction technique that is similar in principle to Soxhlet extraction, but the use of elevated temperature and pressure with ASE allows the extraction to be completed within a short time and with a small quantity of solvent. In this study, we investigated the effect of residue aging, solvent type, and ASE conditions on the recovery of atrazine and alachlor from different soils, and compared the efficiency of ASE with that of Soxhlet and solvent-shake extractions. With ASE, the use of dichloromethane-acetone (1:1, v/v) or methanol as solvent resulted in significantly greater pesticide recovery than hexane. After the residue was aged for >2 weeks, pesticide recovery was significantly influenced by the extraction temperature in ASE vessel, and the recovery increased to  $130-140^{\circ}$ C and then decreased. The efficiency of ASE was generally better than that for Soxhlet or shake extraction using methanol-water (4:1, v/v). ASE extraction also consumed considerably less solvent than the other two conventional methods.

Environ. Sci. Technol. 33:3249-3253, 1999.

### TEMPERATURE AND MOISTURE EFFECTS ON FUMIGANT DEGRADATION IN SOIL

#### J. Gan, S.K. Papiernik, S.R. Yates and W.A. Jury

Recent discovery of the contribution of methyl bromide fumigation to stratospheric ozone depletion has revealed our limited understanding of the environmental processes of fumigants. For instance, little is known about fumigant degradation in soil under high temperature or low moisture conditions that prevail near the soil surface during fumigation. In this study we determined the interaction of soil temperature and moisture with degradation of 1,3-dichloropropene (1,3-D) and methyl isothiocyanate (MITC) for extended soil temperature and moisture ranges. Fumigant degradation increased 5 to 12 times when temperature increased from 20 to 50°C. It was further shown that chemical transformation of fumigants always increased with increasing temperature, but temperature effects on microbial degradation were fumigant dependent. The relative contribution of microbial degradation to the overall fumigant degradation was highest for the soil with highest organic matter content, and was greater for MITC than for 1,3-D isomers. When the temperature was >30°C, microbial degradation of 1,3-D was substantially suppressed, while that of MITC was greatly stimulated. As soil moisture content increased, 1,3-D degradation accelerated, but that of MITC decreased. The specific responses of fumigant degradation to temperature and moisture variations should be considered when describing their transport in the environment, and also may be used for designing fumigation practices that allow reduced atmospheric emissions.

J. Environ. Qual. 28:1436-1441, 1999.

#### ENHANCED FUMIGANT ACITVITY AT HIGHER SOIL TEMPERATURE

#### S.K. Xue, J. Gan, J.O. Becker, S.R. Yates and S.K. Papiernik

In soil solarization, temperature increases are typically the greatest near the soil surface, and gradually diminish with depth. Consequently, soil solarization provides good pest control near the surface, and often inadequate suppression for deep layers. Soil solarization combined with fumigation at regular or reduced rates was found to substantially improve pest control compared to solarization or fumigation alone. The enhanced efficacy was caused by synergistic interactions between fumigants and temperature. Synergistic interactions between fumigants and temperature are potentially useful in that they may be used for designing integrated practices to improve the efficacy of solarization. In particular, if the synergism allows lower rates of fumigants to be used, environmental input of chemical fumigants will also be reduced. So far, however, fumigant-temperature interactions have not been systematically studied. The main objective of this study was to determine the interaction between soil temperature and activities of methyl bromide (MeBr) and 1,3-dichloropropene (1,3-D) against citrus nematode *Tylenchulus semipenetrans*.

Soil (50 g) in 170 mL glass bottles was inoculated with about 600 nematode juveniles extracted from infested citrus roots, and then exposed to MeBr and 1,3-D at 20, 30, 40, and 45°C. After exposure for 6,12,24,48, and 96 h, replicate samples (x 4) were extracted on Baermann funnels and the remaining nematode density was enumerated. Two replicate samples were simultaneously removed for analysis of residual fumigant concentrations. Concentration-time index (ct) was calculated, and correlated with nematode mortality. Soil samples not treated with fumigants also received the same temperature treatments.

In untreated soil, nematode survival was not significantly affected by temperature in the range of 20-30°C, but was strongly reduced at temperature  $\geq$ 40°C. This suggests that temperatures  $\geq$ 40°C were lethal for *Tylenchulus semipenetrans*, while a temperature  $\leq$ 30°C was sublethal. In fumigated soil, nematode suppression was a combined result of fumigant activity and temperature effect. For the same fumigant rate, nematode suppression was closely dependent on the temperature of incubation. Nematode suppression at 40°C in fumigated soils was similar to that in untreated soil, indicating that temperature alone was sufficient to provide the activity. Nematode responses to temperature were different between 20°C and 30°C. In general, much less time was required for the same rate to achieve 100% nematode suppression at 30°C than at 20°C. Likewise, at all levels, after exposure for the same time, greater suppression of nematodes occurred at 30°C than at 20°C. In contrast, in untreated soil, nematode survival was found to be unaffected at 20 and 30°C. This implies that synergistic reaction occurred between temperature and fumigant, which resulted in a higher fumigant activity at 30°C than at 20°C.

Proc. of the Annual Int. Res. Conf. On Methyl Bromide Alternatives and Emissions Reductions. Nov. 1-4, San Diego, CA. 95:1-3, 1999.

### CONCENTRATION- AND TEMPERATURE- DEPENDENT DEGRADATION OF TWO FUMIGANTS IN A SANDY SOIL

#### Q.L. Ma, J. Gan, S.K. Papiernik, J.O. Becker and S.R. Yates

Soil temperature and fumigant concentration on degradation of methyl isothiocyanate (MITC) and 1,3-dichloropropene (1,3-D) in Arlington sandy loam (coarse loam, mixed, thermic, hapllic Duroxeralf) were studied and an inverse first-order model was proposed to describe the concentration-degradation rate relationship. At the same concentration, degradation of MITC and 1,3-D increased with temperature from 20 to 40 C and followed the Arrhenius equation ( $r^2 > 0.81$ ). At the same temperature, degradation rates of both fumigants were inversely proportional to concentration and were well described by an inverse first-order equation ( $r^2 > 0.89$ ). Degradation rates of MITC varied by approximately an order of magnitude in the concentration range of ~3 and 140 mg kg<sup>-1</sup>, depending on temperature. Likewise, degradation rates of (E)1,3-D isomer varied between 2.1 and 4.1 times, and of (Z)-1,3-D isomer between 1.5 and 2.9 times, in the concentration range of 0.6 and 60 mg kg<sup>-1</sup>. It is suggested that pesticide fate models should include both temperature and concentration in simulating dissipation of MITC and 1,3-D in the field.

Agronomy Abstract p. 312, 2000.

#### REDUCE PESTICIDE AIR POLLUTION WITH REACTIVE FERTILIZERS

#### J. Gan and S.R. Yates

Soil fumigants are a class of highly volatile pesticides. They are used in warm regions for treating soils to eradicate soilborne pathogens, nematodes and weeds. Most existing fumigants are halogenated Cl-C3 compounds, including methyl bromide (MB), 1,3-dichloropropene (1,3-D), and chloropicrin (CP). Two more halogenated hydrocarbons, methyl iodide (MI) and propargyll bromide (PB), are currently being investigated as alternatives to MB. These halogenated fumigants share similar properties such as high volatilization potential, high acute toxicity, and potential mutagenicity. These characteristics together suggest that atmospheric emissions of these products may become a significant source of air pollution that can inflict hazardous effects on field workers or nearby residents. Therefore, feasible measures to suppress fumigant emissions are imperatively needed.

We have discovered that these halogenated fumigants can all undergo nucleophilic substitution reaction With thiosulfate salts such as ammonium-, sodium-, potassium-, and calcium thiosulfate. Transformation by thiosulfate greatly decreased the activity of these fumigants, and also converted them into non-volatile dehalogenated anions. We have carried out systematic experiments to develop protocols to use thiosulfate salts for reducing fumigant volatilization from soil. Because many thiosulfate salts are commercial fertilizers and thus available at a low cost, the use of thiosulfate fertilizers to reduce fumigant emissions represents one of the most feasible option. So far we have completed several column experiments and field trials to evaluate reductions of emission achieved by surface amendment of ammonium thiosulfate (ATS), and factors affecting the magnitude of reduction. We report such applications using 1,3-D as an example.

ACS 219th National Meetings in San Francisco, CA, 40(1), 2000.

### COLUMN SYSTEM FOR CONCURRENT ASSESSMENT OF EMISSION POTENTIAL AND PEST CONTROL OF SOIL FUMIGANTS

#### J. Gan, C. Hutchinson, F.F. Ernst, J.O. Becker and S.R. Yates

Fumigation for soilborne pest and pathogen control is under close scrutiny because of its potential hazardous effects on the environment and on human health. Therefore, reduced-risk yet effective fumigation practices are imperatively needed. We have developed a column system that allows an integrated evaluation of emission potential and efficacy of fumigants. The system consists of a large, packed soil column and a sampling chamber for measuring fumigant emissions at the soil surface. Nematodes (or other pests) can be inoculated into the column and their survival may be assayed after the treatment. This approach was used to evaluate the emission of 1,3-dichloropropene (1,3-D) and its efficacy against the citrus nematode *Tylenchulus semipenetrans* when ammonium thiosulfate, a 1,3-D degrading fertilizer, was applied at the soil surface. Results closely comparable to field observations were obtained. Compared with field studies, the proposed method is rapid and inexpensive, and thus may be used for screening fumigation practices that have improved environmental safety and pest control performance.

J. Environ. Qual. 29:657-661, 2000.

### DEGRADATION AND VOLATILIZATION OF THE FUMIGANT CHLOROPICRIN AFTER SOIL TREATMENT

J. Gan, S.R. Yates, F.F. Ernst and W.A. Jury

Chloropicrin (CP) is used in fumigation of soil-borne pests. Because of its high volatility and toxicity, atmospheric emission of CP during soil application may become a source of air pollution. We investigated degradation of CP in three different soils as a function of soil temperature and moisture conditions, and evaluated its volatilization against methyl bromide (MeBr) from packed soil columns. Chloropicrin degraded much faster than MeBr in the same soil, mainly via microbial degradation. Degradation of CP accelerated as soil temperature increased, but was relatively independent of changes in soil moisture. When the soil surface was uncovered, overall volatilization loss of CP was similar to that of MeBr. Covering the soil surface with a polyethylene or high-barrier film was much more effective in reducing volatilization of CP than MeBr. Therefore, surface covers may be used in sensitive areas to reduce human exposure to CP.

J. Environ. Qual. 29:1391-1397, 2000.

### TEMPERATURE AND MOISTURE EFFECTS ON FUMIGANT DEGRADATION IN SOIL

#### J. Gan, S.K. Papiernik, S.R. Yates and W.A. Jury

Recent discovery of the contribution of methyl bromide fumigation to stratospheric ozone depletion has revealed our limited understanding of the environmental processes of fumigants. For instance, little is known about fumigant degradation in soil under high temperature or low moisture conditions that prevail near the soil surface during fumigation. In this study we determined the interaction of soil temperature and moisture with degradation of 1,3-dichloropropene (1,3-D) and methyl isothiocyanate (MITC) for extended soil temperature and moisture ranges. Fumigant degradation increased 5 to 12 times when temperature increased from 20 to 50°C. It was further shown that chemical transformation of fumigants always increased with increasing temperature, but temperature effects on microbial degradation were fumigant dependent. The relative contribution of microbial degradation to the overall fumigant degradation was highest for the soil with highest organic matter content, and was greater for MITC than for 1,3-D isomers. When the temperature was >30°C, microbial degradation of 1,3-D was substantially suppressed, while that of MITC was greatly stimulated. As soil moisture content increased, 1,3-D degradation accelerated, but that of MITC decreased. The specific responses of fumigant degradation to temperature and moisture variations should be considered when describing their transport in the environment, and also may be used for designing fumigation practices that allow reduced atmospheric emissions.

J. Environ. Qual. 28:1436-1441, 1999.

### SURFACE APPLICATION OF AMMONIUM THIOSULFATE TO REDUCE 1,3-DICHLOROPROPENE VOLATILIZATION FROM SOIL

#### J. Gan, J.O. Becker, F.F. Ernst, C. Hutchinson, J.A. Knuteson and S.R. Yates

Atmospheric emission of the soil fumigant 1,3-dichloropropene (1,3-D) is of environmental concern because of its toxicity and carcinogenicity. Thiosulfate fertilizers were previously found to rapidly transform 1,3-D to non-volatile, less toxic ions in soil. In this study, we investigated the use of surface application of ammonium thiosulfate (ATS) for reducing 1,3-D volatilization. In packed soil columns, 1,3-D emission decreased with increasing ATS application rate and the amount of water used for delivering ATS. When ATS was applied in 9 mm water at 64 g m², total 1,3-D emission was reduced by 61%. The reduction increased further to 89% when ATS was applied at 193 g m². Bioassays showed that ATS application did not affect 1,3-D's effectiveness for controlling inoculated citrus nematodes. In field plots where 1,3-D was applied via subsurface drip, surface spray of ATS reduced 1,3-D emissions by 50% when the soil surface was not tarped, and by 71% when the surface was tarped with polyethylene sheets. ATS application had no effect on the efficacy of root-knot nematode control or tomato yields. These results suggest that surface application of thiosulfate fertilizers is a feasible and effective strategy for minimizing 1,3-D emissions, and should be further explored.

Pest. Management Science 56:264-270, 2000.

### TRANSFORMATION OF 1,3-DICHLOROPROPENE IN SOIL BY THIOSULFATE FERTILIZERS

#### J. Gan, S.R. Yates, J.A. Knuteson and J.O. Becker

The pesticide 1,3-dichloropropene (1,3-D) is considered to be the most promising alternative to methyl bromide for soilborne pest control. The high volatility of 1,3-D, however, has been shown to result in excessive atmospheric emissions that may impose toxicological effects on workers or residents. This study demonstrated that 1,3-D was rapidly transformed to nonvolatile products by thiosulfate fertilizers in soil, and that thiosulfate-facilitated fumigant transformation may be used to reduce 1,3-D emissions. Transformation of 1,3-D by thiosulfate was chemically based, and 1,3-D degradation in soil accelerated proportionally as thiosulfate level in soil increased. At a 4:1 thiosulfate to fumigant molar ratio, the half-life of 1,3-D was reduced to only a few hours, as compared with > 10 d for nonamended soils. The rate of thiosulfate-facilitated 1,3-D transformation was independent of soil types and was higher in moist soils and at high soil temperatures. Transformation occurred at a similar rate for ammonium, calcium, and sodium thiosulfates. As these thiosulfate compounds are commercial fertilizers, amendment of these products at the soil surface during 1,3-D fumigation may offer an effective and inexpensive approach for reducing 1,3.D emissions.

J. Environ. Qual. 29:1476-1481, 2000.

### NEMATODE RESPONSE TO METHYL BROMIDE AND 1,3-DICHLOROPROPENE SOIL FUMIGATION AT DIFFERENT TEMPERATURES

#### S.K. Xue, J. Gan, S.R. Yates and J.O. Becker

Several heat-based methods, such as soil solarization, are being developed as alternative practices for managing soilborne pests and pathogens. The effectiveness of these practices is often inconsistent or marginal, thus commanding the need for their integration with other methods. The main objective of this study was to determine synergistic interaction between soil fumigants and temperature. Citrus nematode *Tylenchulus semipenetrans* infested soil was exposed to methyl bromide (MeBr) or 1,3-dichloropropene (1,3-D) at various temperatures. Fumigant degradation was concurrently measured and concentration-time index (ct) were calculated and correlated to the recovered nematode population. In untreated soil, nematode survival was not affected from 20 to 30°C, but was strongly reduced at  $\geq$  40°C. In fumigated soil, nematode suppression was much greater at 30°C than at 20°C, and the ct required for nematode elimination at 30°C was only <50% of that needed at 20°C for both fumigants. These results suggest that these fumigants became more active with increasing temperature in the sub-lethal temperature range. It also implies that when integrated with a heat-based practice, reduced rates of fumigants may provide adequate pest control, thus minimizing the environmental input of chemical fumigants.

Pest Management Science 56:737-742, 2000.

### ADSORPTION AND CATALYTIC HYDROLYSIS OF DIETHATYL-ETHYL ON HOMOIONIC CLAYS

W.P. Liu, J.

#### Gan, S.K. Papiernik and S.R. Yates

Adsorption and catalytic hydrolysis of the herbicide diethatyl-ethyl [N-chloroacetyl-N-(2,6-diethylphenyl)glycine ethyl ester] on homoionic Na $^+$ , K $^+$ -, Ca $^{2+}$ -, and Mg $^{2+}$ - montmorillonite clays were studied in aqueous media. The Freundlich adsorption coefficient, Kf, measured from isotherms on clay followed the order of Na $^+$   $\approx$  K $^+$ > Mg $^{2+}$   $\approx$  Ca $^{2+}$ . Analysis of FT-IR spectra of diethatyl-ethyl adsorbed on clay suggests probable bonding at the carboxyl and amide carbonyl groups of the herbicide. The rate of herbicide hydrolysis in homoionic clay suspensions followed the same order as that for adsorption, indicating that adsorption may have preceded and thus caused hydrolysis. Preliminary product identification showed that hydrolysis occurred via nucleophilic substitution at the carboxyl carbon, causing the cleavage of the ester bond and formation of diethatyl and its dechlorinated derivative, and at the amide carbon, yielding an ethyl ester derivative and its acid. These pathways also suggest that hydrolysis of diethatyl-ethyl was catalyzed by adsorption on the clay surface.

J. Agric. Food Chem. 48:1935-1940, 2000.

### STRUCTURAL INFLUENCES IN RELATIVE SORPTIVITY OF CHLOROACETANILIDE HERBICIDES ON SOIL

#### W. Liu, J. Gan, S.K. Papiernik and S.R. Yates

Adsorption of the chloroacetanilide herbicides acetochlor, alachlor, metolachlor and propadhlor was determined on soils and soil components, and their structural differences were used to explain their sorptivity orders. On all soils and soil humic acids, adsorption decreased in the order: metolachlor > acetochlor > propachlor > alachlor. On Ca-saturated montmorillonite, the order changed to metolachlor > acetochlor > propachlor. FT-IR differential spectra of herbicide-clay or herbicide-hurnic acid-clay showed possible formation of hydrogen bonds and charge transfer bonds between herbicides and adsorbents.. The different substitutions and their spatial arrangement in the herbicide molecule were found to affect the relative sorptivity of these herbicides by influencing the reactivity of functional groups participating in these bond interactions. It was further suggested that structural differences of pesticides from the same class may be used as a molecular probe to obtain a better understanding of adsorption mechanisms of pesticides on soil.

J. Agric. Food Chem. 48:4320-4325, 2000.

#### EFFECTS OF COMPONENT INTERACTIONS ON HERBICIDE ADSORPTION

#### J. Gan, W.P. Liu, S.K. Papiernik and S.R. Yates

Pesticide adsorption on soil is known to depend closely on organic matter (OM) and clay compositions. Adsorption in OM-clay mixtures, however is often significantly less than the sum of adsorption on the individual components, suggesting component interaction results in modified adsorption behavior. We determined adsorption of a few acetanilide herbicides in mixtures of humic acid (HA) and montmorillonite. As the ratio of HA to clay increased, Kd first decreased and then increased, but was always smaller than what might be estimated by assuming independent adsorption. A mathematical relationship was developed to describe this phenomenon. The deviation from independent adsorption varied also with the type of herbicide and the interacting time between the adsorbing components. It is likely that the interaction changed the available adsorption sites, and thus the overall adsorption.

Agronomy Abstract p. 336, 1999.

### ASSESSMENT AND EMISSION REDUCTION OF METHYL BROMIDE ALTERNATIVE FUMIGANTS

#### J. Gan, S.R. Yates, J.O. Becker and W.A. Jury

The imminent phase-out of methyl bromide (MeBr) has stimulated an intensive search for alternatives. Chemical alternatives to MeBr include 1,3dichloropropene, methyl isothiocyanate, chloropicrin, methyl iodide, and propargyl bromide. These compounds are all highly volatile and toxic, and some are carcinogenic. Their emissions into the air during use may impose great risks to workers and residents. This project aims to evaluate emission potential of these fumigants under typical application practices, to understand factors that influence their volatilization, and to develop feasible measures to reduce their emissions. We have so far obtained a systematic understanding of fumigant behavior such as transformation and transport, and identified variables that control emission. This information will be used for assessing the relative environmental hazard of different fumigants, and for designing safer fumigation practices.

Agronomy Abstract p. 365, 1999.

#### PESTICIDES PARTITIONING IN A CREEPING BENTGRASS PUTTING GREEN

#### L. Wu. R. Green, M.V. Yates, J. Gan, S.R. Yates and G. Liu

Turfgrass is one the most intensively managed biotic systems in the urban landscape. The purpose of this study was to determine the fate of four pesticides (chlorothalonil, metalaxy, chlopyrifos, and trichlorfon) when applied to turfgrass in an environment that closely resembles golf-course conditions. Partitioning of the four pesticides in a creeping bentgrass (Agrostis palustris Huds.) putting green was monitored for volatilization loss, clipping removal, leaching below the root-zone, and distribution in the soil profile. Results showed that volatilization mainly occurred at the initial period after pesticide application. The total amount of volatilization was in the range of 0.01 to 2.8% of the applied pesticides. Clipping removal was very small, ranging from 0.03 to 0.21 %. Under normal management practices, pesticide leaching was minimal. The cumulative leaching was less than 0.003% of the applied pesticides. Most of the applied pesticides remained in the surface 2 cm of the profile, where they subjected to rapid degradation.

Agronomy Abstract p. 52, 2000.

#### INHIBITION OF ADSORPTION ON PESTICIDE REMEDIATION IN SOIL

#### J. Gan, Q. Wang, S.K. Papiernik and S.R. Yates

Benign chemical transformations can be used to remove organic contaminants from soil. The effectiveness of using such transformations for soil remediation, however, is affected by the adsorption of the contaminant to soil, as adsorption renders the target contaminant inaccessible for the reaction. We studied the influence of soil type and  $K_{\rm d}$  on the transformation rate of a number of pesticides by thiosulfate salts. For non-adsorbing pesticides such as halogenated fumigants, transformation rate was not greatly affected by soil type and the reaction proceeded almost as rapidly as in the aqueous phase. For adsorbing species such as chloroacetanilide herbicides, transformation rate was negatively correlated with the  $K_{\rm d}$  value and was especially slow in organic matter-rich soils. This dependence suggests that the effectiveness of soil remediation using chemical reactions would be soil- and contaminant-dependent, and may not be directly extrapolated from the reaction rate in the aqueous phase.

Agronomy Abstract p. 388, 2000.

### DOSE-RESPONSE RELATIONSHIPS BETWEEN METHYL ISOTHIOCYANATE AND BARNYARD GRASS SEEDS IN A SOIL AT DIFFERENT TEMPERATURES

#### Q.L. Ma, J. Gan, J.O. Becker, S.K. Papiernik and S.R. Yates

Temperature and fumigation rates on germination of barnyard grass seeds (Echinochloa crus-galli) were studied to evaluate the effectiveness of weed management at a reduced fumigation rate and elevated temperature. Fresh soil mixed with the weed seeds was treated with methyl isothiocynate (MITC) at a range of concentrations and then incubated at 20, 30, and 40°C. Samples were taken periodically to determine MITC concentration and weed germination rate. With no fumigation weed germination rate was not significantly affected by temperature between 20 and 40°C. When combined with fumigation, germination rate was significantly reduced. At 7% of the recommended application rate, the time required to inhibit 50% of the germination rate ( $T_{50}$ ) was 68.4, 17.9 and 8.7 h at 20, 30 and 40°C, respectively. At the same temperature,  $T_{50}$  value decreased significantly with increasing fumigation rate. However, the product of dose C and exposure time (T) for 50% of inhibition in germination rate (CT50) was not a constant. A large C resulted in a small CT50 value, and vise versa. The results provide scientific bases for applying impermeable plastic films on soil surface as the films increase the soil temperature and also keep a higher fumigant concentration.

Agronomy Abstract p. 319, 2000.

# IMPACTS OF METHYL BROMIDE AND ITS ALTERNATIVES ON SOIL MICROBIAL COMMUNITIES

### A.M. Ibekwe, S.K. Papiernik, J. Gan, S.R. Yates, D. Crowley and C.H. Yang

Soil fumigation is the primary method used in reducing soilborne plant pathogens and parasitic nematodes that cause severe damages to high value crops in the warm region of the U.S. It is often required to reduce root-knot nematode populations. The fumigants methyl bromide (MeBr), 1,3-dichloropropene (1,3-D), methyl isothiocyanate (NHTC), and chloropicrin are known to have broad biocidal activity, and their effects on soil bacteria are largely unknown. Recently, the effect of MITC (the toxic degradation product of metam sodium) on soil bacterial population structure and function was studied by the use of traditional heterotrophic activity measures, and biochemical assays. The long-term goal of the research in our laboratory in response to the EPA action is to evaluate new or existing alternative fumigants for control of soilborne plant pathogens to replace methyl bromide in high value crop areas. Biologically-based and environmentally-safe alternatives, such as compost amendment and biosolid application, are being investigated for possible use in integrated management strategies for accelerated degradation of fumigants. The hypothesis governing this practice is that organic amendments, when applied to soil, add different substrates that can be used by soil bacteria for growth. However, soils are fumigated by direct injection into the subsurface soil with little or no surface litter. The impacts of this practice on soil microorganisms have rarely been shown. The impact of fumigants on soil microorganisms is being evaluated in view of their role in sustaining the global cycling of matter and their function in supporting soil quality for productive agriculture. In this paper, we describe the effect of MeBr, NHTC, 1,3-D and chloropicrin on soil microbial population in a laboratory microcosm experiment. Our objectives were to monitor the biocidal effects of these fumigants and compare their ecological effects on soil microorganisms in response to fumigation at recommended application rates. To overcome the drawbacks of studying the effect on individual bacterial strains, since only about 1% of total bacteria in the soil can be cultured, we used the nucleic acid approach by employing different PCR methods to analyze the total bacterial population in our samples. We also used biochemical and metabolic approaches to evaluate how microorganisms respond to certain carbon substrates after fumigation. We used the Biolog system in this study to monitor functional changes by heterotrophs and PLFA/DNA fingerprinting to quantify microbial biomass and community diversity composition. Since microbial biomass as determined by PLFA is based on the relationship between the phylogerry of microorganisms and their PLFA profiles, we believe that the use of PLFA techniques provides an unbiased description of the effects of fumigants on microbial population. This allowed us to interpret the effect of fumigants on different groups of bacteria fungi, and actinomycetes. The total bacterial DNA fingerprinting by denaturing gradient gel electrophoresis (DGGE) provided a complete picture on the effects of these compounds on the dominant bacterial populations. Through this we calculated the structural diversity of the microbial community. This provided distinct diversity value for each sample and we were able to observe changes in bacteria composition over the 12 week study period.

Proceedings of the 1999 Annual International Research Conference on Methyl Bromide Alternatives and Emissions Reductions. November 1-4, San Diego, CA. 96:1-3, 1999.

### IMPACTS OF FUMIGANT TREATMENT ON SOIL MICROBIAL COMMUNITIES BY DGGE

A.M. Ibekwe, S.K. Papiernik, J. Gan, S.R. Yates, D. Crowley and C.H. Yang

The ability of soil microbial communities to rebound after shock treatment from fumigants is critical to the sustainability of agricultural ecosystems. Culture- independent approaches, namely, PLFA and DGGE were used to determine changes in soil microbial community structure in a microcosm, experiment following application of MeBr, MITC, 1,3-D and chloropicrin. Similarity among the different 16S rDNA profiles from fumigated soil was quantified by analyzing the DGGE band patterns. The Shannon index of diversity H was calculated for each fumigated soil sample. High diversity index was maintained between the control soil and the different fumigants, except Methyl bromide (H decreased from 1.11 to 0.13). After 12 wk incubation, H increased to 0.63 in the methyl bromide treated samples. PCA of PLFA profiles showed that microbial communites from methyl bromide treated soil may be different from other soils treated with other fumigants.

Agronomy Abstract p. 224, 1999.

### MICROCOSM ENRICHMENT OF FUMIGANT-DEGRADING SOIL MICROBIAL COMMUNITIES

M. Ibekwe, S.K. Papiernik, J. Gan, S.R. Yates, C.H. Yang and D. Crowley

DGGE profiles of PCR amplified 16S rDNA genes were used to assess the diversity of fumigant-adapted microbial communities. Growth of microorganisms was stimulated by incubating soil with or without organic amendment and different fumigants in glass columns. After 6 months, stable population densities of fumigant degrading communities were established and a large percentage were able to grow on fumigant-containing minimal medium plates. DGGE provided a fast evaluation of the distribution of amplified sequence types. The banding patterns from samples treated with organic amendment and fumigants were different from the control soil. Fragments from 26 individual DGGE bands were sequenced and compared to published 16S rRNA gene sequences. Our results suggest that application of organic amendment with fumigants may enhance growth of specific strains of bacteria that can increase the degradation rate of these compounds.

Agronomy Abstract p. 225, 1999.

## IMPACT OF FUMIGANTS OF STRUCTURAL DIVERSITY OF AMMONIA-OXIDIZING BACTERIA

#### A.M. Ibekwe, S.K. Papiernik, J. Gan and S.R. Yates

Ammonia-oxidizing bacteria perform the first step in nitrification, which is known to be the rate-limiting step. To determine the effects of fumigants on nitrification rates and on community structure of ammonia-oxidizing bacteria, a microcosm approach was used in a 12 wk incubation experiment with soil that has no history of fumigation. The data suggest that nitrification was significantly disrupted after the first 7 d of the experiment. The effects were more severe with MeBr and MITC treatments than with 1,3-D and chloropicrin. The community structures of ammonia-oxidizing bacteria from the four treatments were compared by 16S rDNA PCR-DGGE analysis using primers that target this group. DGGE analysis of ammonia oxidizing bacteria from the four treatments revealed two identical bands with the primers, indicating spatial and temporal reproducibility after 12 wk. Sequencing of these clones revealed the presence of only Nitrosospira-like sequences. Southern blot analysis with the primers showed a very bright band of correct size with Nitrosospira probe in all the treatments after 8 wk, but not with Nitrosomonas probe.

Agronomy Abstract p. 256, 2000.

## SPATIAL AND TEMPORAL DISTRIBUTION OF SOIL BORON CONTENT IN SELECTED IRRIGATED SOILS

### J.A. Jobes, P.J. Shouse, S. Goldberg, J.E. Ayars and R. Soppe

Boron is an important micro-nutrient for plant growth, but the range between sufficiency and toxicity is reportedly narrow for agronomic crops. We surveyed several soils using various extraction methods to determine the spatial and temporal distributions of extractable Boron and salinity in California. The extraction methods gave similar trends, but the absolute concentrations were quite different. The relationships among the extractable Boron and plant uptake are being studied and results will be presented. Our geostatistical results indicate that the overall variance in Boron concentration is higher at shallow depths and lower at depth in soils that have shallow groundwater. Boron concentrations are correlated with salinity and the correlations were stronger with depth. Boron and salinity were relatively constant during our study (3-5 years).

Agronomy Abstract p. 217, 2000.

## CHARACTERIZATION AND MEASUREMENT OF THE UNSATURATED POROUS MEDIA

### F.J. Leij and M. Th. van Genuchten

Quantifying and elucidating fluid flow in partially saturated porous media remains an important challenge, with many scientific and management applications. This paper contains a synopsis of theoretical and experimental methods to study and estimate the hydraulic properties of unsaturated media. Our main purpose is to provide a framework for the Proceedings of the workshop "Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media." We first discuss some of the problems related to the characterization and modeling of fluid flow in unsaturated media, as well as recent progress in this area. Subsequently we will peruse contributions to the workshop along five broad themes: (i) pore-scale phenomena, including those for multifluid systems, (ii) direct measurement methods, (iii) inverse modeling, (iv) indirect methods, and (v) other contributions pertaining to recent flow and transport research. We conclude by listing a number of topics in need for further investigation; this following a similar list compiled after the previous workshop [van Genuchten and Leij, 1992].

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 1-12, University of California, Riverside, CA, 1999.

#### PRINCIPLES OF SOLUTE TRANSPORT

### F.J. Leij and M. Th. van Genuchten

The chapter reviews elementary aspects of solute transport in soils. Such transport has traditionally been described with the convection-dispersion equation (CDE). This equation incorporates two constitutive transport processes: (i) movement as a result of liquid flow and (ii) spreading as a result of known and unknown processes such as diffusion and small scale variations in the water flow velocity. In Part II we will review several modes of solute transport: convection, diffusion in free liquids and subsequently in soils, mechanical dispersion, and (hydrodynamic) dispersion. The governing transport equation is derived from mass balance principles in Part III. Many other processes may affect the movement and fate of solutes in soils. Part IV is devoted to the important process of linear and nonlinear solute adsorption.

*In*: J. van Schilfgaarde and W. Skaggs (ed.), *Drainage in Agriculture*, Chapter 9, pp. 331-359, Agronomy No. 38, Am. Society of Agronomy, Madison, WI, 1999.

#### SOLUTE TRANSPORT

#### F.J. Leij and M. Th. van Genuchten

The topic of solute transport in soils was reviewed in a general manner in this chapter. The description focused on the use of the advection-dispersion equation (ADE). The key concepts for transport according to the ADE were introduced with a brief discussion of how to determine transport parameters. The development and, especially, the application of process-based models to field- and laboratory-scale transport is likely to remain of great importance for studying and managing the fate and movement of chemicals in soils. Such models are attractive because they may yield information for a much wider range of conditions than can be achieved through regular experimental investigations. Most attention hence was paid to formulating transport models.

The successful application of a transport model requires that the water flow regime can be quantified. This can usually be done prior to solving the transport problem but in some cases the solute regime will affect the soil hydraulic properties. Diffusion, which is included in the dispersive term of the ADE, may become an important mechanism for solute movement in the liquid phase in soils with low water velocities. The difference in terminology regarding tortuosity was brought up in section 6.2. 1. 1, which also contained some background on diffusion measurements. Mechanical dispersion, or simply dispersion, has been widely discussed in the literature and an introduction was provided to the subject in section 6.2.1.2. The ADE was subsequently formulated using the principle of mass conservation. The movement of the solute may be greatly affected by adsorption onto the solid phase. Linear and nonlinear adsorption were therefore discussed in the context of solute transport modeling. Multicomponent transport was very briefly reviewed in section 6.2.4 because the behavior of a single solute species in a natural soil will usually be affected by many different components and a variety of chemical processes. Particularly for flow and transport in natural soils, the ADE should account for nonequilibrium transport. Nonequilibrium transport may occur during solute movement in structured media with bypass flow or for kinetic solute adsorption. Section 6.2.5 contains the mathematical formulation for a bi-continuum nonequilibrium model as well as an analytical solution and application for solute input to a structured soil.

Analytical and numerical modeling of the ADE was discussed in section 6.3. This section specified relevant concentration modes as well as boundary and initial conditions needed to complete the mathematical formulation of the transport problem. Analytical solutions may be useful to gain further insight in the transport model, to study solute behavior in soils over large temporal or spatial scales, to evaluate numerical models, and to determine model parameters from results of well-controlled experiments. Various transformations were provided that facilitate such solutions and selected equilibrium and nonequilibrium solutions were provided. Applications of these solutions were also illustrated. Time moments were defined for describing the breakthrough and spreading of a solute in soils as an alternative to the standard solution of the governing partial differential equations for solute transport. A general overview was given of numerical solution procedures for the ADE with a qualitative outline was included of the common methods of finite differences and finite elements. The finite difference method is attractive because of its simplicity while the finite element method is better able to handle a solution domain with an irregular geometry or nonuniform transport properties. The effect of the numerical scheme on the predicted concentration profile was shown for a relatively large column Peclet number.

Stochastic modeling of (field-scale) transport of chemicals in soils is increasingly receiving

attention in the literature because of soil heterogeneity, limitations in the invoked transport models, and uncertainty in the estimated transport parameters. The stream tube concept is one of a few stochastic approaches that can be applied to actual problems. The stream-tube model simplifies the heterogeneity of the soil and allows the use of analytical techniques to estimate the averaged concentration across the field as well as its variation for specified probability density functions for

*In*: M. Sumner (ed.), *Handbook of Soil Science*, Chapter 6, pp. A183-1227. CRC Press, Boca Raton, FL, 1999.

selected transport parameters.

# RELATIONSHIP BETWEEN PARTICLE-SIZE DISTRIBUTION AND SOIL WATER RETENTION

### L.M. Arya, F.J. Leij and M. Th. van Genuchten

The water retention characteristic of a soil is intimately related to its particle-size distribution and packing density. Translation of the particle-size distribution into a corresponding soil water characteristic curve involves converting particle sizes to equivalent pore radii, and solid mass fractions to equivalent pore volumes. Since particle sizes are expressed in diameters of equivalent spheres, the simplest geometrical structure is one in which uniform-size spherical particles are arranged in cubic close-packed assemblages. The pore lengths and pore radii in such hypothetical cubic structures can be scaled to those in corresponding natural structures, made up of the same solid mass but consisting of nonspherical particles in random orientations. The procedure involves measuring the natural pore length in units of the number of spherical particles, with each particle contributing a length equal to its diameter. Thus, if the *i*th particle-size fraction consists of  $n_i$  spherical particles of radius  $R_i$ , tracing the pore length generated by the fraction solid mass, when arranged in a natural state of packing, would require  $n_i^{\alpha}$  particles of radius  $R_i$ . The concept first developed by Arya and Paris [1981] treated  $\alpha$  as a universal constant. In this study,  $\alpha$  is defined for individual particle-size fractions according to  $\alpha_i = (\log N_i / \log n_i)$ , where  $N_i = n_i^{\alpha}$ . Our study, applied to five textural classes, shows that  $\log N_i$  is related to  $\log n_i$  following a logistic growth equation and that  $\alpha$  is not a constant; rather  $\alpha$  decreases with increasing particle size. However, the decrease in  $\alpha$  is relatively small from clayto medium sand-size particles. A sharp decrease in  $\alpha$  occurs only for relatively coarse particles. The new formulation for  $\alpha$  and the constant average values calculated for various textural classes were evaluated for 23 soils, presenting a range of particle-size distribution, bulk density, and organic matter content. The general shape of the soil water characteristic curves could be predicted fairly well with both forms of  $\alpha$ , with the predicted pressures differing from the experimental pressures by no more than what might be expected between random samples of the same soil. However, the single-value average  $\alpha$  consistently predicted lower pressures in the wet range and higher pressures in the dry range, thereby showing a pronounced bias in the predictions. The new formulation for  $\alpha$ produced closer agreement with the experimental data, and no bias was observed.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 931-946, University of California, Riverside, CA, 1999.

# RELATIONSHIP BETWEEN THE HYDRAULIC CONDUCTIVITY FUNCTION AND THE PARTICLE-SIZE DISTRIBUTION

#### L.M. Arya, F.J. Leij, P.J. Shouse and M. Th. van Genuchten

We present a model to compute the hydraulic conductivity, K, as a function of water content,  $\theta$ , directly from the particle-size distribution (PSD) of a soil. The model is based on the assumption that soil pores can be represented by equivalent capillary tubes and that the water flow rate is a function of pore size. The pore-size distribution is derived from the PSD using the Arya-Paris model. Particle-size distribution and  $K(\theta)$  data for 16 soils, representing several textural classes, were used to relate the pore flow rate and the pore radius according to  $q_i = cr_i^x$  where  $q_i$  is the pore flow rate (cm³ s¹) and  $r_i$  is the pore radius (cm). Log c varied from about -2.43 to about 2.78, and x varied from  $\approx 2.66$  to  $\approx 4.71$ . However, these parameters did not exhibit a systematic trend with textural class. The model was used to independently compute the  $K(\theta)$  function, from the PSD data for 16 additional soils. The model predicted  $K(\theta)$  values from near saturation to very low water contents. The agreement between the predicted and experimental  $K(\theta)$  for individual samples ranged from excellent to poor, with the root mean square residuals (RMSR) of the log-transformed  $K(\theta)$  ranging from 0.616 to 1.603 for sand, from 0.592 to 1.719 for loam, and from 0.487 to 1.065 for clay. The average RMSR for all textures was 0.878.

Soil Sci. Soc. Am. J. 63(5):1063-1070, 1999.

### SCALING PARAMETER TO PREDICT THE SOIL WATER CHARACTERISTIC FROM PARTICLE-SIZE DISTRIBUTION DATA

### L.M. Arya, F.J. Leij, M. Th. van Genuchten and P.J. Shouse

The Arya-Paris model is an indirect method to estimate the soil water characteristic from particle-size data. The scaling parameter,  $\alpha$ , in the original model was assumed constant for all soil textures. In this study, at is defined as  $\alpha = (\log N/\log n_i)$ , where  $n_i$  is the number of spherical particles in the ith particle-size fraction (determined by the fraction solid mass, w, and mean particle radius,  $R_i$ ) and  $N_i$  is the number of spherical particles of radius  $R_i$ , required to trace the pore length generated by the same solid mass in a natural structure soil matrix. An estimate for  $\log N_i$  was obtained by either relating  $\log N_i$  to  $\log n_i$  using a logistic growth equation or by relating  $\log N_i$  linearly to  $\log (w/R_i^3)$  based on the similarity principle. For any given texture, both approaches showed that a was not constant but decreased with increasing particle size, especially for the coarse fractions. In addition,  $\alpha$  was also calculated as a single-value average for a given textural class. The three formulations of  $\alpha$  were evaluated on 23 soils that represented a range in particle-size distribution, bulk density, and organic matter content. The average  $\alpha$  consistently predicted higher pressure heads in the wet range and lower pressure heads in the dry range. The formulation based on the similarity principle resulted in bias similar to that of the constant α approach, whereas no bias was observed for the logistic growth equation. The logistic growth equation implicitly accounted for bias in experimental procedures, because it was fitted to  $\log N_i$  values computed from experimental soil water characteristic data. The formulation based on the similarity principle is independent of bias that might be inherent in experimental data.

Soil Sci. Soc. Am. J. 63(3):510-519, 1999.

#### STOCHASTIC MODEL FOR POST-TILLAGE SOIL PORE SPACE EVOLUTION

#### D. Or, F.J. Leij, V. Snyder and T.A. Ghezzehei

Tillage operations disrupt surface layers of agricultural soils, creating a loosened structure with a substantial proportion of interaggregate porosity that enhances liquid and gaseous exchange properties favorable for plant growth. Unfortunately, such desirable soil tilth is structurally unstable and is susceptible to change by subsequent wetting and drying processes and other mechanical stresses that reduce total porosity and modify pore size distribution (PSD). An ability to model post-tillage dynamics of soil pore space and concurrent changes in hydraulic properties is important for realistic predictions of transport processes through this surface layer. We propose a stochastic modeling framework that couples the probabilistic nature of pore space distributions with physically based soil deformation models using the Fokker-Planck equation (FPE) formalism. Three important features of soil pore space evolution are addressed: (1) reduction of the total porosity, (2) reduction of mean pore radius, and (3) changes in the variance of the PSD. The proposed framework may be used to provide input to hydrological models concerning temporal variations in near-surface soil hydraulic properties. In a preliminary investigation of this approach we link a previously proposed mechanistic model of soil aggregate coalescence to the stochastic FPE framework to determine the FPE coefficients. An illustrative example is presented which describes changes in interaggregate pore size due to wetting-drying cycles and the resulting effects on dynamics of the soil water characteristic curve and hydraulic conductivity functions.

Water Resour. Res. 36(7):1641-1652, 2000.

## PREDICTING UNSATURATED HYDRAULIC CONDUCTIVITY FUNCTIONS FROM PARTICLE SIZE DISTRIBUTIONS

### L.M. Arya, F.J. Leij, P.J. Shouse and T.H. Skaggs

We present a model to compute the hydraulic conductivity-water content function directly from the particle size distribution of a soil. The model is based on the assumption that soil pores can be represented by equivalent capillary tubes and that the water flow rate is a function of pore size. Particle size distribution and conductivity data for 16 soils were used to relate the pore flow rate to the pore radius. Parameters of this logarithmic function did not exhibit a systematic trend with textural class. The model was used to compute the hydraulic conductivity for 16 additional soils. The agreement between the predicted and the experimental values for individual samples ranged from excellent to poor with the root mean square residuals of the log transformed conductivity ranging from 0.62 to 1.60 for sands, from 0.59 to 1.72 for loams and from 0.49 to 1.07 for clays. The average root mean square residuals for all textures was 0.88.

Agronomy Abstract p. 193, 1999.

#### SCALING HYDRAULIC PROPERTIES OF A MACROPOROUS SOIL

#### **B.P.** Mohanty

Macroporous soils exhibit significant differences in their hydraulic properties for different pore domains. Multimodal hydraulic functions may be used to describe the characteristics of multiporosity media. I investigated the usefulness of scaling to describe the spatial variability of hydraulic conductivity (K(-h)) functions of a macroporous soil in Las Nutrias, New Mexico. Piecewise-continuous hydraulic conductivity functions suitable for macroporous soils in conjunction with a hybrid similar media-functional normalization scaling approach were used. Results showed that gravity-dominated flow and the related hydraulic conductivity (K(-h)) functions of the macropore region are more readily scalable than capillary-dominated flow properties of the mesopore and micropore regions. A possible reason for this behavior is that gravity-dominated flow in the larger pores is mostly influenced by the pore diameter, which remains more uniform as compared to tortuous mesopores and micropores with variable neck and body sizes along the pore length.

Water Resour. Res. 35(6):1927-1931, 1999.

#### SOIL MOISTURE CONTENT AT DEEPER DEPTHS - SGP971 OKLAHOMA

#### B.P. Mohanty, P.R. Houser, P.J. Shouse and M. Th. van Genuchten

The soil moisture content at deeper depths is important for global water balance calculations. While recent developments of remote sensing technologies seem more tractable for estimating the soil moisture content (SMC) of relatively shallow depths (0-5 cm) over large land areas, numerical variably-saturated flow modeling provides an attractive tool for extrapolating surface SMCs to deeper depths. In this paper we show results of HYDRUS model simulations at several locations across the Southern Great Plains Hydrology Experiment 1997 (SGP97) region. HYDRUS is based on the one-dimensional Richards equation for variably-saturated flow, and the van Genuchten functions for soil water retention and unsaturated hydraulic conductivity. The model can handle both flux- and head-type boundary conditions, root water uptake, and temperature dependent as well as hysteretic soil hydraulic properties. Atmospheric forcing such as transient precipitation (flux) provide the top boundary condition for water flow simulations in one-dimensional soil pedons. Observed gravimetric SMC data measured during SGP97 at deeper depths (up to 1 m) at several locations using a truck-mounted Giddings probe were used to test the model predictions. A reasonable match between observed and simulated SMCs were noted at several quarter sections with different soil textures. SMCs at deeper depths in the fields with grass/wheat cover were equally well predicted as bare land. Contrary to common perception, the one-dimensional model even performed reasonably well at the sampling points having moderate slopes.

Proc. 14th Conf. On Hydrology, American Meteorological Society, Boston, MA, pp. 141-142, 1999.

#### SCALING BEHAVIOR OF NEAR-SATURATED HYDRAULIC CONDUCTIVITY

#### B.P. Mohanty and P.J. Shouse

The near-saturated hydraulic conductivity function, K(h), is critical for describing flow in macropores and other structural voids. The usefulness of similar media scaling and functional normalization to describe the near-saturated hydraulic conductivity function, K(h), measured *in situ* at 296 spatial locations across a heterogenous agricultural field was tested. Disc (ponded and tension) infiltrometers were used to measure K(h) at different field positions (corn row, no traffic inter-row, and traffic inter-row) cutting across different soil types (Nicollet and Clarion loam derived from glacial till material). The K(h) data ranged several orders of magnitude for different field positions and soil types and were found to be statistically different between different field positions. Using a Gardner type K(h) function, relative hydraulic conductivity values, and a hybrid of similar media scaling and functional normalization concepts all disc infiltrometer data sets were coalesced to a single reference curve. A novel finding is that saturated hydraulic conductivities ( $K_{sat}$ ) could be successfully used as the scale factor for the near-saturated K(h) functions (e.g., 0-15 cm soil water tension) under all field positions and soil types at the experimental field.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, Part 1, pp. 1415-1424, University of California, Riverside, CA, 1999.

# INTER-COMPARISON OF THREE METHODS FOR MEASURING SOIL MOISTURE DURING SGP97

#### R.L. Elliott, P.R. Houser and B.P. Mohanty

Soil moisture plays a major role in the physics of the soil-plant-atmosphere continuum. Soil moisture is a key factor in plant growth, evapotranspiration, soil water and heat flux, and the hydrologic and surface energy balances. The water content of soils influences rainfall-runoff relationships, flooding potential, ground water recharge, and biological processes. Effective drought assessment and irrigation management are dependent on soil moisture information. round-based soil-moisture measurement was an integral part of the Southern Great Plains 1997 (SGP97) Hydrology Experiment, and was particularly focused on providing "ground truth" information for remote sensing techniques (Jackson, 1999; Humes et al., 1999). Near-surface and profile measurements of soil moisture were made using a variety of techniques and instrumentation. These data were inter-compared and quality assured to maximize their value in meeting the Experiment's objectives.

Our study used three independent sources of SGP-97 soil moisture information: (1) surface and profile measurements of gravimetric water content; (2) measurements of volumetric water content using time domain reflectometry; and (3) heat dissipation sensors for measuring soil matric potential, installed at four depths. Each technique yields a different unit of measurement for soil moisture, so conversions must be made before the data can be inter-compared.

Reprints, 14<sup>th</sup> Conference on Hydrology, pp. 178-181. American Meteorological Society, Boston, MA. 1999.

## GROUND-BASED INVESTIGATION OF SOIL MOISTURE VARIABILITY WITHIN REMOTE SENSING FOOTPRINTS DURING SGP97: FIRST RESULTS

J.S. Famiglietti, J.A. Devereaux, C. Laymon, T. Tsegaye, P.R. Houser, T.J. Jackson S.T. Graham, M. Rodell and B.P. Mohanty

The Southern Great Plains 1997 (SGP97) Hydrology Experiment was the largest airborne L-band passive microwave mapping mission of surface soil moisture to date. Located in a 50 km by 250 km strip of central Oklahoma, soil moisture was mapped nearly every day between June 18 and July 18, 1997, at a 1-km ground resolution. Since the hydrologic community anticipates that the SGP97 sensor, the ESTAR (Electronically Scanned Thinned Array Microwave Radiometer), will ultimately provide 25-50 km resolution global soil moisture monitoring from a space-based platform, the goal of this investigation was to more rigorously characterize ESTAR performance than would be possible with a standard, ground-truth sampling plan typically associated with soil moisture remote sensing experiments. Specifically, the goal of this field investigation was to provide, to the degree possible given the constraints of the SGP97 experiment, accurate estimates of the mean, variance, and frequency distributions of surface moisture content within selected, representative, sensor footprints. Ongoing research will compare our observations to ESTAR-derived soil moisture field values, with implications for ESTAR accuracy and the underlying variability that remote sensing cannot record explicitly (i.e. the variance and frequency distributions).

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 563-570, University of California, Riverside, CA, 1999.

# THE SPATIAL-TEMPORAL STRUCTURE OF U.S. SOUTHERN GREAT PLAINS SOIL MOISTURE: AN ANALYSIS OF IN-SITU PROFILE OBSERVATIONS

#### P.R. Houser and B.P. Mohanty

Soil moisture links the hydrologic cycle and the energy budget of land surfaces by regulating the partitioning of surface radiative energy between latent and sensible eat fluxes. Therefore, accurate assessment of the spatial and temporal variation of soil moisture is important for the study, understanding, and management of surface biogeophysical processes. However, soil moisture exhibits a high degree of variability whose cause has been elusive, but is thought to be determined by heterogeneity in soil properties, vegetation, topography, water table depth, precipitation, and other meteorological factors. Understanding and assessment of these variations across a range of scales will enable the definition of the vertical and horizontal soil moisture error correlation structures which are essential for soil moisture assimilation studies.

During the Southern Great Plains Experiment (SGP97) (Jackson, 1997), soil moisture, soil properties, vegetation characteristics, and meteorological information was measured for a period of 30 days at a wide range of scales ranging from 1 m to 250 km. The preliminary analysis of these observations is presented here. This analysis is focused on the calibration of soil moisture measurements and assessment of the spatial and temporal structure of soil moisture at El Reno, Oklahoma.

The Delta-T frequency domain reflectometer Theta Probes used in this study to measure near-surface soil moisture showed little inter-probe variability, and some soil dependence. The ESI time domain reflectometer Moisture Point Probes used to measure profile soil moisture over several depth ranges generally overestimate soil moisture, with a decreasing sensitivity with depth. It is suspected that soil heterogeneity and compression adversely influence both the Theta and Moisture Point Probes. In the analysis of near-surface soil moisture sampling error, it was found that both average sampling error, and soil moisture variability increase in drier soil. Sampling error is also generally scale independent. There is a high degree of uncorrelated soil moisture spatial variability both horizontally and vertically, although some spatial structure is evident.

Preprints, 14<sup>th</sup> Conference on Hydrology, pp. 204-205, American Meteorological Society, Boston, MA, 1999.

## SPATIO-TEMPORAL EVOLUTION AND TIME STABILITY OF SOIL MOISTURE CONTENT DURING THE SGP97 HYDROLOGY EXPERIMENT

### B.P. Mohanty and T.H. Skaggs

Air-borne passive microwave remote sensors measure soil moisture at the footprint scale, a scale of several hundred square meters or kilometers that encompasses different characteristic combinations of soil, topography, vegetation, and climate. Studies of within-footprint variability of soil moisture are needed to determine the factors governing hydrologic processes and their relative importance, as well as to test the efficacy of remote sensors. We used gridded ground-based impedance probe water content date and aircraft mounted Electronically Scanned Thinned Array Radiometer (ESTAR) pixelaverage soil moisture data to investigate the spatio-temporal evolution and time stable characteristics of soil moisture in three selected (LW03, LW13, LW21) footprints from the Southern Great Plains 1997 (SGP97) Hydrology Experiment. Better time stable features were observed within a footprint containing sandy loam soil than within two pixels containing silty loam soil. Additionally, flat topography with split wheat/grass land cover produced the largest spatio-temporal variability and the least time stability in soil moisture patterns. A comparison of ground-based and remote sensing data showed that ESTAR footprint-average soil moisture was well calibrated for the LW03 pixel with sandy loam soil, rolling topography, and pasture land cover, but improved calibration is warranted for the LW13 (silty loam soil, rolling topography, pasture land) and LW21 (silty loam soil, flat topography, split vegetation of wheat and grass land with tillage practice) pixels. Footprint-scale variability and associated nonlinear soil moisture dynamics may prove to be critical in the regional-scale hydroclimatic models.

Am. Geophys. Union, p. 553, 2000.

# EVOLUTION OF SOIL MOISTURE SPATIAL STRUCTURE IN A MIXED VEGETATION PIXEL DURING THE SOUTHERN GREAT PLAINS 1997 (SGP97) HYDROLOGY EXPERIMENT

### B.P. Mohanty, J.S. Famiglietti and T.H. Skaggs

Different factors contribute to soil-moisture variability at different space scales and time scales, including soil properties, topography, vegetation, land management, and atmospheric forcings, such as precipitation and temperature. Field experiments supported by adaptive geostatistical and exploratory analysis, including categorical elimination of different governing factors, are needed to bring new insight to this important hydrologic problem. During the Southern Great Plains 1997 (SGP97) Hydrology Experiment in Oklahoma, we investigated the within-season (intra-seasonal) spatiotemporal variability of surface (0 - 6 cm depth) soil moisture in a. quarter section (800 m x 800 m) possessing relatively uniform topography and soil texture but variable land cover. Daily soil moisture measurements were made between June 22 and July 16 using portable impedance probes in a regular 7 x 7 square grid with 100-m spacings. Initially, the land cover was split between grass and wheat stubble; row tilling on June 27 converted the wheat stubble to bare ground. Geostatistical and median polishing schemes were used to analyze the within-season evolution of the spatial structure of soil moisture. The effects of daily precipitation, variable land cover, land management, vegetation growth, and micro-heterogeneity including subgrid-scale variability were all visible in the analysis. The isotropic spatial correlation range for soil moisture varied between <100 m (for nugget and subgrid-scale variability) and >428 m (for spherical and Gaussian models) within the 4-week-long SGP97 experiment. The findings will be useful for assessing remotely sensed soil moisture data collected during the SGP97 Hydrology Experiment in mixed vegetation pixels.

Water Resour. Res. 36(12):3675-3686, 2000.

# ANALYSIS AND MAPPING OF FIELD-SCALE SOIL MOISTURE VARIABILITY USING HIGH-RESOLUTION, GROUND-BASED DATA DURING THE SOUTHERN GREAT PLAINS 1997 (SGP97) HYDROLOGY EXPERIMENT

#### B.P. Mohanty, T.H. Skaggs and J.S. Famiglietti

Soil moisture is an important state variable in the hydrologic cycle, and its spatiotemporal distribution depends on many geophysical processes operating at different spatial and temporal scales. To achieve a better accounting of the water and energy budgets at the land-atmosphere boundary, it is necessary to better understand the spatiotemporal variability of soil moisture under different hydrologic and climatic conditions and at different hierarchical space scales and timescales. During the Southern Great Plains 1997 (SGP97) Hydrology Experiment the 0-6 cm soil water content was measured on consecutive afternoons at 400 locations in a small, gently sloping range field (Little Washita field site 07). The soil moisture measurements were made using portable impedance probes. Spatiotemporal data analyses of the two sampling events showed a significant change in the field variance but a constant field mean, suggesting moisture was redistributed by (differential) base flow, evapotranspiration, and condensation. Among the different relative landscape positions (hilltop, slope, valley) the slope was the largest contributor to the temporal variability of the soil moisture content. Using a sequential aggregation scheme, it was observed that the relative position influencing the field mean and variance changed between the two sampling events, indicating time instability in the spatial soil moisture data. Furthermore, high-resolution (impedance probe) sampling and limited (gravimetric) sampling gave different field means and variances.

Water Resour. Res. 36(4):1023-1031, 2000.

# WATER AND CHLORIDE TRANSPORT IN A FINE-TEXTURED SOIL: FIELD EXPERIMENTS AND MODELING

### D. Ventrella, B.P. Mohanty, J. Šimůnek, N. Losavio and M. Th. van Genuchten

Numerical models are being used increasingly to simulate water and solute movement in the subsurface for a variety of applications in research and soil/water management. Although a large number of models of varying degrees of complexity have been developed over the years, relatively few have been tested under field conditions. We tested the performance of the HYDRUS-1D computer model to simulate variably saturated water flow and chloride transport in a fine-textured Italian soil subject to a fluctuating saline groundwater table. The model was also used for estimating solute transport parameters using an inverse optimization scheme. Our results indicate that including the effects of immobile water produced better predictions of chloride transport compared with the traditional convection-dispersion transport approach. Including anion exclusion as well did not improve the model predictions appreciably. Occasional deviations between model prediction and field observation were attributed to unrepresented lateral groundwater flow processes and to preferential flow through macropores or other structural voids. The HYDRUS-ID model was found to be very useful for analyzing the relatively complex flow and solute transport processes 'at our field site and for estimating model parameters using inverse procedures.

Soil Sci. 165:624-631, 2000.

# MODELING PREFERENTIAL FLOW IN A TILE-DRAINED FIELD USING DOUBLE-HUMP TYPE K(H) FUNCTIONS

### **B.P.** Mohanty

Preferential flow under saturated as well as near-saturated conditions through macropores, cracks, and other non-matrix domains that coexist with the soil matrix domain, has been found to be very common in structured field soil. Disc infiltrometry methods involving ponded and tension infiltrometers in conjunction with multi-step outflow methods could provide a more complete *K-h* function for field soils. Results of a flow-transport field study near Las Nutrias, New Mexico will be summarized in this presentation. A novel finding of this study is the (bimodal) double-hump feature of the measured *K-h* function, which was modeled using piecewise-continuous functions. Incorporating the bimodal *K-h* functions in a numerical model (CHAIN\_2D) improved the flow and transport predictions at the field site. Furthermore, *K-h* functions for gravity-dominated flow regions were found to be more readily scalable than *K-h* functions for capillary-dominated flow regions.

Agronomy Abstract p. 194, 1999

#### SORPTION OF FUMIGANTS TO AGRICULTURAL FILMS

#### S.K. Papiernik, J. Gan, J.A. Knuteson and S.R. Yates

Plastic tarps are often used in soil fumigation to contain chemicals in the soil to increase efficacy and decrease emissions of fumigant vapors. This research has shown that plastic films have a significant capacity to sorb fumigant vapors and that the sorption is largely reversible. We tested three agricultural films (polyethylene and two high barrier films) with four soil fumigants (methyl bromide, chloropicrin, 1,3-dichloropropene, and propargyl bromide, a potential alternative to methyl bromide). We observed significant sorption of all fumigants to all the films at field relevant concentrations. Partition coefficients (sorbed/vapor-phase concentration) ranged from <1 dm³/m².film for methyl bromide to ~200 dm³/m² film for chloropicrin. Sorption isotherms were linear, indicating that the film may be a large sink for fumigant vapors. Sorption of most fumigants was very rapid, with the bulk of the sorption occurring within the first few minutes of contact. Desorption was also rapid, with most desorption occurring within minutes after the film samples were removed to fresh air. First-order rate constants for desorption were -0.5 to 1.5 min¹. Sorption/desorption may be important in reducing emissions and determining worker exposure and should be considered in measurements involving agricultural films.

Environ. Sci. Technol. 33:1213-1217, 1999.

# A NEW METHOD FOR ESTIMATING THE PERMEABILITY OF PLASTIC FILMS TO FUMIGANT VAPORS

### S.K. Papiernik and S.R. Yates

When greenhouse and field soils are fumigated, the soil surface is often covered with a plastic tarp to reduce loss of the chemical via volatilization. Low- or high-density polyethylene tarps (LDPE or HDPE) are commonly used; however, these films have been reported to have signficant permeability to methyl bromide (MeBr) and other soil fumigants. Plastic films that have reduced permeability to soil fumigants, particularly MeBr, have been developed in response to the call for management practices that reduce emissions and maintain or increase the efficacy of soil fumigants. To assist in the development of these management practices, a rapid, accurate method to measure the permeability of plastic films to soil fumigants is needed. The permeability of plastic films to gaseous solutes is due to diffusion and is thought to occur by the solute dissolving into the surface of the film, followed by the diffusion through the film and evaporation from the opposite film surface. This paper describes a new method for estimating the mass transfer coefficient of gases diffusing through plastic films. Unlike currently-used methods, which use a flow-through chamber under steady state conditions, the transfer of fumigant across a film was determined in a static chamber. This method was used to measure the permeability of HDPE to MeBr, 1,3-dichloropropene (1,3-D), and chloropicrin.

Permeability cells were fabricated from stainless steel cylindrical stock of 12 cm ID. Cells were constructed in two halves, each approximately 4 cm long, sealed on one end by soldering a stainless steel plate to the column. Additional cells for the testing of low permeability films were 12 cm (H) x 1 cm (each half). A piece of the plastic film to be tested was placed between the two cell halves and the cell halves sealed together to provide a gas tight system. Sampling ports were constructed from brass fittings and were installed at the midpoint of each cell half.

Vapor was spiked on one side of the film (source chamber), and the gas-phase concentration on each side of the film was monitored until concentrations in the source chamber and receiving chamber were equal. MeBr, 1,3-D, and chloropicrin were spiked to separate cells (3 replicates per fumigant). Gas-tight syringes were used to collect vapor samples from each chamber at various times throughout the course of the experiment. Samples were placed in headspace vials and analyzed using headspace GC-ECD.

Proceedings of the 1999 Annual International Research Conference on Methyl Bromide Alternatives and Emissions Reductions. November 1-4, San Diego, CA. 3 0:1-3, 1999.

### PRESENCE AND BIOTRANSFORMATION OF THREE HETEROAROMATIC COMPOUNDS COMPARED TO AN AROMATIC HYDROCARBON

# J. Hellou, J. Leonard, J. Meade, S. Sharpe, J. Banoub, S.K. Papiernik, L. Eglinton and J. Whelan

The presence of nitrogen, oxygen and sulfur containing aromatic compounds, namely carbazole, dibenzofuran. dibenzothiophene and their alkylated derivatives was investigated in potential environmental sources of these compounds. The persistence vs biodegradation of the parental heteroaromatic compounds was determined using bacterial consortia collected from three marine beaches from coastal Newfoundland. Experiments were performed at 25 and 4°C and bacterial populations derive from differently contaminated environments. In separate studies, rainbow trout, Salmo gardneiri, were exposed to PACs through their diet and the bioelimination of crlucuronide and sufate conjugates followed in the gall bladder bile after a single and during continuous exposure. Comparison was done between the presence and fate of the three heterocyclic PACs and that of fluorene. a PAH counterpart with similar structure and physicalchemical properties. The tissue distribution of the PACs (not presented). provides information on the potential narcotic and/or reproductive effect of the unreacted compounds and the metabolites on the potential toxicity of the oxidation products.

Polycyclic Aromatic Compounds 14:221-230, 1999.

# A REVIEW OF IN SITU MEASUREMENT OF ORGANIC COMPOUND TRANSFORMATION IN GROUNDWATER

### S.K. Papiernik

Laboratory assessments of the rate of degradation of organic compounds in groundwater have been criticized for producing unrepresentative results. The potential for organic compounds to be transformed in groundwater has been measured using in situ methods, which avoid problems of attempting to duplicate aquifer conditions in the laboratory. In situ assessments of transformation rates have been accomplished using transport studies and in situ microcosms (ISMs); a review of these methods is given here. In transport studies, organic solutes are injected into an aquifer and the concentrations are monitored as they are transported downgradient. The change in mass of a solute is determined by the area contained under the breakthrough curve (plot of concentration versus time). ISMs isolate a portion of the aquifer from advective flow and act as in situ batch reactors. Experiments using ISMs involve removing water from the ISM, amending it with the solutes of interest, re-injecting the amended water, and monitoring the solute concentrations with time. In both transport and ISM studies, the loss of organic solutes from solution does not allow for a distinction between sorptive, abiotic and biotic transformation losses. Biological activity can be chemically suppressed in ISMs and the results from those experiments used to indicate sorption and abiotic loss. Transformation products may be monitored to provide additional information on transformation mechanisms and rates.

Third SETAC World Congress, May 21-25, Brighton, UK, 2000.

#### PRODUCTS OF PROPARGYL BROMIDE DEGRADATION IN SOIL

#### S.K. Papiernik, J. Gan, R. Dungan and S.R. Yates

Propargyl bromide (C3H3Br; PrBr) is being investigated for its potential to partially replace methyl bromide (MeBr) as a soil finnigant. Information on its environmental fate, including mechanisms of degradation in soil, is required to evaluate PrBr's capacity for sustained usage. We have conducted a number of studies on the degradation on PrBr in soil, and monitored the formation of some of the products of PrBr degradation in soil and water.

Primary alkyl halides, including MeBr and PrBr react via nucleophilic substitution. This reaction mechanism imparts broad-spectrum toxicity through alkylation of nucleophilic groups in amino acids and peptides. All known mechanisms of PrBr and MeBr degradation in soil and water result in the formation of Br. Analysis of additional degradation products gives information on the mechanism of transformation.

Proceedings of the 2000 Annual International Research Conference on Methyl Bromide Alternatives and Emissions Reductions. November 6-9, Orlando, FL. 27-1-3, 2000.

# MECHANISM OF DEGRADATION OF METHYL BROMIDE AND PROPARGYL BROMIDE IN SOIL

### S.K. Papiernik, J. Gan and S.R. Yates

The degradation of methyl bromide (MB) and propargyl bromide (PB) was investigated in soil and water to obtain information on the mechanism of degradation. It has been suggested that primary alkyl halides (including MB and the potential alternatives PB and methyl iodide) can undergo SN2 nucleophilic substitution with nucleophilic sites on soil organic matter (i.e., -NH2, -NH, -OH, -SH). The pattern of product formation observed in this study provides more direct evidence that fumigants that are primary alkyl halides can alkylate soil organic matter and that this may be a significant mechanism of degradation in soil. Degradation in water samples (hydrolysis) formed Br and the corresponding alcohol (propargyl alcohol from PB, methanol from MB) in equimolar amounts. The rate of hydrolysis was not significantly different from the rate of Br formation for both MB and PB. Degradation in two soils resulted in the formation of Br, but very little production of the corresponding alcohol, indicating that some mechanism other than hydrolysis must be occurring in the soil. Degradation of MB and PB was much more rapid in the higher organic-matter day loam soil than in the sandy loam soil. Spiking <sup>14</sup>C-labeled MB to soil resulted in the formation of nonextractable (soilbound) <sup>14</sup>C, which increased as the extractable <sup>14</sup>C decreased. Microbial oxidation was not significant in these soil samples, which were sterilized through autodaving and/or treatment with high concentrations of fumigants. These results provide further experimental evidence that MB, PB, and similar compounds can alkylate soil organic matter.

J. Environ. Qual. 29:1322-1328, 2000.

#### PERMEABILITY OF PLASTIC FILMS TO FUMIGANT VAPORS

### S.K. Papiernik and S.R. Yates

When greenhouse and field soils are fumigated, the soil surface is often covered with a plastic tarp to reduce loss of the chemical via volatilization. Polyethylene tarps are commonly used; however, these films have significant permeability to methyl bromide and other soil fumigants. Films with lower permeability are being introduced. To develop management practices that protect the environment while providing adequate pest control, a rapid, accurate method to measure the permeability of plastic films to soil fumigants is needed. This paper describes a new method for estimating the mass transfer coefficient of agricultural films. The time-dependent transfer of fumigant across a membrane was determined in a static chamber; this method was used to measure the permeability of several plastic films to methyl bromide and other fumigants. This method, which requires a minimum of equipment, is especially useful as a screening tool in the development of new plastics, soil fumigants, and management practices.

Agronomy Abstract p. 33, 1999.

#### HERBICIDE-SALINITY INTERACTION EFFECTS ON PHYTOTOXICITY

### S.K. Papiernik, C.M. Grieve, J. Gan, F.F. Ernst and S.R. Yates

The potential for irrigation water salinity to impact herbicide phytotoxicity to soybeans and six weed species was tested in a greenhouse study. Seeds were germinated and grown in individual pots irrigated with Hoagland's nutrient solution or simulated saline drainage water (EC 7dS/m) supplemented with nutrients. Imazethapyr (Pursuit, 4 oz/ac) and chlorimuron ethyl (Classic, 0.5 oz/ac) were applied post-emergence according to the label directives. Control plants were treated with the tank mix containing no herbicide. Plant growth was monitored for several weeks following herbicide application. In general, plants irrigated with saline water had a poorer germination rate, grew more slowly, and had a lower survival rate than plants grown using non-saline irrigation water. However, for some herbicide-plant type combinations, particularly with chlorimuron ethyl, no difference in post-treatment growth between the two water conditions was observed and salinized plants exhibited similar or higher survival rates. Strong differences in plant development were observed in herbicide-treated and control plants, with no observable effect of salinity. Herbicide treatment apparently disrupted the apical meristem of several species, including soybeans, with the subsequent formation of multiple shoots at the growing point; often one shoot became dominant and the plant partially recovered.

Agronomy Abstract p. 142, 2000.

## DEVELOPMENT AND USE OF A HIERARCHICAL SET OF NEURAL NETWORK PEDOTRANSFER FUNCTIONS

#### M.G. Schaap, F.J. Leij and M. Th. van Genuchten

Pedotransfer functions (PTFs) are increasingly being used to obtain soil hydraulic characteristics for local, regional and global scale hydrological problems. In many cases, estimates by PTFs are simply indispensable because of the sheer cost and effort involved with direct measurements of the hydraulic characteristics. We will present a hierarchical system of PTFs based on neural network and bootstrap analyses and address several important issues. Data sets used for calibration of PTFs may contain many predictors which can be used to improve the accuracy of PTFs. However, in most hydrological studies not all required input variables may be available. To address this problem we developed a hierarchical set of five PTFs to make optimal use of limited or more extended sets of available predictors. Because all five PTFs were developed using the same data set, the predictions with the different models are consistent among each other. Besides striving for maximum accuracy and usability of PTFs, quantification of uncertainty of predicted values is also an important issue. We demonstrate that the uncertainty of PTF predictions depend not only upon the number of predictors, but also on the data that were used for calibration. The hierarchical set of PTFs is implemented in the program Rosetta (available at www.ars.usda.gov) which allows the prediction of water retention, saturated and unsaturated hydraulic conductivity. We will demonstrate the hierarchical approach using data from an IGBP initiative that provides soil hydraulic properties for the FAO soil map of the world. Finally, we will address some unresolved issues, such as the discrepancy between "structural" and "matrix" saturated hydraulic conductivities.

Am. Geophys. Union, p. 370, 1999.

# A BOOTSTRAP-NEURAL NETWORK APPROACH TO PREDICT SOIL HYDRAULIC PARAMETERS

#### M.G. Schaap, F.J. Leij and M. Th. van Genuchten

Indirect estimation using pedotransfer PTFs of soil hydraulic properties has long received considerable attention. PTFs use regressions to predict soil hydraulic parameters from surrogate data such as soil texture and bulk density. Ideally, PTFs should provide both accurate predictions as well a measure of the reliability of those predictions. Most reviews of PTFs have focused on the accuracy, in terms of how well a particular PTF predicts hydraulic parameters of an independent data set. The reliability of PTF predictions can be quantified using the probability distribution of a prediction. Such information, normally not available, is strongly dependent upon the distribution of data in the original calibration data set. In this paper we present information about the use of a combined bootstrap-neural network procedure to predict water retention parameters, the saturated and unsaturated hydraulic conductivity, and their associated probability distributions. We also present user-friendly software that implements the developed neural-network pedotransfer functions.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization* and Measurement of the Hydraulic Properties of Unsaturated Porous Media, Part 1, pp. 1237-1250, University of California, Riverside, CA, 1999.

# COMPARISON OF PEDOTRANSFER FUNCTIONS TO COMPUTE WATER HOLDING CAPACITY USING THE VAN GENUCHTEN MODEL FOR INORGANIC SOILS

#### B. Imam, S. Sorooshian, T. Mayr, M.G. Schaap, H. Wosten and B. Scholes

Three different PTFs, which are used to predict parameters of the van Genuchten model, were compared using a large number of soil samples obtained from the ISRIC data set. The studied models included two regression type models developed by Wosten (the WSC mdoel) and Mayr (the SSLRC model) and one neural network model developed Schaap (USSL-NN). The comparison criterion consisted of calculating several quantitative measures of performance that are capable of addressing systematic errors, unsystematic errors, and total errors. Using observed and predicted values of the water content at several points on the theoretical pF curve, these performance measures were computed and compared for the entire sample as well as for several stratifications of the sample. The stratified study was conducted to assess the sensitivity of model performance to soil characteristics under the assumption that the robustness of each model and its applicability to a wide range of soils can be identified by assessing the sensitivity of its performance measures to soil characteristics. Throughout the comparative study, the USSL-NN model was superior both in overall performance and in sensitivity, particularly with respect to the two critical pressure levels 1/3 bar and 15 bar, both of which were selected as the default values defining water holding capacity.

Report to the IGBP-DIS soils data tasks, IGBP-DIS working paper #22. IGBP-DIS office, CNRM, Toulouse Cedex, France, 1999.

#### CHARACTERIZATION OF SOIL HYDRAULIC PARAMETER UNCERTAINTY

#### P.D. Meyer, G.W. Gee, M.L. Rockhold and M.G. Schaap

Uncertainty in predictions of contaminant transport in the environment can be significant, particularly when these predictions must be based on limited site-specific data and relatively simple models. This paper discusses the use of indirect estimation methods and large soils databases in deriving probability distributions for soil hydraulic parameters. Such distributions can be used to represent the uncertainty in model parameters. The potential effect of the type of input data used in the indirect estimation method was explored using a hierarchical neural network approach. Input to the neural networks included (1) percent sand, silt, and clay, (2) the three textural measurements plus bulk density, and (3) the textural measurements, bulk density, and water content at 33 kPa. Outputs were the parameters of the van Genuchten water retention model. Results indicate that the hydraulic parameter distributions become more representative as the amount of input data increased. The parameter distributions resulting from the neural networks were also compared to distributions from a multiple regression model. A Bayesian approach is also presented for updating soil hydraulic parameter probability distributions using site-specific data. An example illustrates the application of the method. Five site-specific estimates of the water retention parameters were used to update generic parameter probability distributions. The effect of the site-specific data on the updated net infiltration was found to be significant.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 2, pp. 1439-1451, University of California, Riverside, CA, 1999.

#### ESTIMATION OF THE SOIL HYDRAULIC PROPERTIES

### M.G. Schaap, F.J. Leij and M. Th. van Genuchten

Many vadose zone studies use numerical models to simulate the movement of water and solutes in the subsurface. Knowledge about the soil hydraulic properties (for example, the water retention curve, and the saturated and unsaturated hydraulic conductivities) is essential for running most or all of these models. A broad array of methods currently exists to determine soil hydraulic properties. In the field or in the laboratory. Field methods allow for in-situ determination of the hydraulic properties but have uncertainties about the actual sample volume. Laboratory measurements require more sample preparation but do allow a larger number of measurements and a better control of the experimental conditions. Most laboratory and field techniques, however, have specific ranges of applicability with respect topsoil type and saturation. Another limitation of direct measurements is that they generally require a substantial investment in both time and money. Also, many vadose zone studies are concerned with large areas of land that may exhibit significant lateral and vertical spatial variability in the soil hydraulic properties. Performing measurements in these cases is virtually impossible, thus requiring alternative methods for estimating soil hydraulic properties. A large number of indirect methods to generate soil hydraulic properties are now also available. Although these techniques very widely in terms of methodology and complexity, all use some form of surrogate data to estimate soil hydraulic properties. In broad terms, three methods can be distinguished: pore-size distribution models, inverse methods and pedotransfer functions. This paper reviews these three types of indirect methods.

*In*: B. B. Looney and R. W. Falta (eds.), *Vadose Zone Science and Technology Solutions*, vol. 1, pp. 501-509, Battelle Press, Columbus, OH, 2000.

### IMPROVED PREDICTION OF UNSATURATED HYDRAULIC CONDUCTIVITY WITH THE MUALEM-VAN GENUCHTEN MODEL

### M.G. Schaap and F.J. Leij

In many vadose zone hydrological studies, it is imperative that the soil's unsaturated hydraulic conductivity is known. Frequently, the Mualem-van Genuchten model (MVG) is used for this purpose because it allows prediction of the unsaturated hydraulic conductivity from water retention parameters. For this and similar equations, it is often assumed that a measured saturated hydraulic conductivity  $(K_s)$  can be used as a matching point  $(K_0)$  while a factor  $S_e^{\perp}$  is used to account for pore connectivity and tortuosity (where  $S_e$  is the relative saturation and L = 0.5). We used a data set of 235 soil samples with retention and unsaturated hydraulic conductivity data to test and improve predictions with the MVG equation. The standard practice of using  $K_0 = K_s$  and L = 0.5 resulted in a root mean square error for  $\log(K)$  (RMSE<sub>k</sub>) of 1.31. Optimization of the matching point ( $K_0$  and L to the hydraulic conductivity data yielded a RMSE<sub> $\kappa$ </sub> of 0.41. The fitted  $K_0$  were, on average, about one order of magnitude smaller than the measured  $K_s$ . Furthermore, L was predominantly negative, casting doubt that the MVG can be interpreted in a physical way. Spearman rank correlations showed that both  $K_0$  and L were related to van Genuchten water retention parameters and neural network analyses confirmed that  $K_0$  and L could indeed be predicted in this way. The corresponding RMSE<sub>k</sub> was 0.84, which was half an order of magnitude better than the traditional MVG model. Bulk density and textural parameters were poor predictors, while addition of K<sub>s</sub> improved the RMSE<sub>k</sub> only marginally. Bootstrap analysis showed that the uncertainty in predicted unsaturated hydraulic conductivity was about one order of magnitude near saturation and larger at lower water contents.

Soil Sci. Soc. Am. J. 64(3):843-851, 2000.

#### PARAMETER CORRELATION STRUCTURES OF HYDRAULIC FUNCTIONS

#### M.G. Schaap and FJ. Leij

Knowledge of the statistical distribution of soil hydraulic parameters and their correlation structure is important for uncertainty analyses of water and solute transport in soils. Many studies use pedotransfer functions (PTFs) to estimate soil hydraulic properties. However, besides providing reliable predictions of hydraulic parameters, it is also important that the PTFs represent the correlation structure in the original data. We fitted various retention equations and unsaturated conductivity models to hydraulic data and examined their parameter correlations as well as those with texture and bulk density. Results for the Mualem-van Genuchten model showed that the matching point and tortuosity parameters were correlated with retention parameters, but that they exhibited only weak relations with texture. Newly developed PTFs preserve the correlation structure present in the fitted parameters and estimated unsaturated conductivity within 0.8 order of magnitude of error.

Agronomy Abstract p. 191, 1999.

# EVALUATION OF EXISTING AND SITE-SPECIFIC PEDOTRANSFER FUNCTIONS TO PREDICT HYDRAULIC PROPERTIES FOR HANFORD SITE SEDIMENTS

#### M.G. Schaap and P.D. Meyer

The safety of current and future storage methods for radioactive waste at the Hanford waste disposal site will be assessed with conceptual models that simulate the hydrological processes in and around the disposal facilities. Presently, the appropriateness of the models is being tested using data obtained in past and recent on-site field experiments. Complicating factors are the depth of the unsaturated zone and the high degree of vertical variability in the sediments (fine sands to gravel), resulting in a high degree of spatial variability in hydraulic properties. One of the tasks is to test whether the required saturated and unsaturated hydraulic data need to be measured, or can be estimated using pedotransfer functions (PTFs). We compare the performance of an existing nation-wide PTF (Rosetta), and site-specific PTFs that were calibrated using data derived from measurements on Hanford sediments (bore holes at the 200 EW sites). An independent test was carried out for data derived from the ILAW site. The first analyses show mixed results. Predictions of water retention parameters with site-specific PTFs have generally higher correlations with independent data than predictions by the general PTF. However, when the same PTFs were evaluated on measured water contents directly, there was little difference in performance. It appears that the general PTF predicts the saturated and unsaturated conductivity much better than the site-specific PTFs. We note, however, that the currently available hydraulic data for Hanford is relatively sparse - affecting both the reliability of the sitespecific PTFs and testing results. Incorporation of data from recent experiments will probably lead to better site-specific PTFs.

Am. Geophys. Union Abstracts, p. 411, 2000.

### APPLICATION OF TDR AND FREQUENCY ANALYSIS TO STUDY THE CALCIC-SODIC STATUS OF A SOIL

#### M.G. Schaap, I. Lebron and D.L. Suarez

A change from a calcium-saturated to a sodic exchange complex often results in a marked decrease in the saturated hydraulic conductivity of soils. This reduction is probably caused by smaller pore sizes due to an increased double layer spacing resulting in the collapse of aggregates. We hypothesize that the collapse of aggregates and the formation of colloids occurs with an increase of the amount of bound water. Because bound water molecules are rotationally hindered, they have different dielectric properties than free water molecules. By determining changes in the frequency dependent dielectric spectrum, we may be able to monitor a change from a calcic to a sodic soil. We subjected a calcic soil to solutions of increasing SAR (sodium absorption ratio) and measured the saturated hydraulic conductivity as an indicator of structural collapse. We measured high-resolution TDR waveforms, which were processed with Fourier analyses to obtain scatter functions and frequency-dependent dielectric properties. Initial analyses show that instrumental difficulties sometimes make it difficult to interpret the results. Reasonable results can be obtained at low frequencies that probably show the most pronounced effects of bound water.

Agronomy Abstract p. 230, 2000.

### ESTIMATES OF SOIL NITRATE DISTRIBUTIONS USING COKRIGING WITH PSEUDO-CROSSVARIOGRAMS

#### R. Zhang, P.J. Shouse and S.R. Yates

Nitrate (NO<sub>3</sub>·) is one of the major nonpoint source pollutants in the vadose zone. In this study, NO<sub>3</sub>· distributions were estimated in an 800 by 800 by 1.8 m soil volume using kriging and cokriging with nonsymmetric pseudo-crossvariograms. Cokriging with pseudo-crossvariograms maximized the use of available information at different soil depths. Cokriging allowed easily obtained information at shallow layers to be used to improve soil chemical estimations at deeper layers. Compared with kriging, cokriging significantly reduced the mean squared errors (MSEs) and mean kriging variances (MKVs) of the NO<sub>3</sub>· estimations in the soil. For the same estimation accuracy of kriging, cokriging with pseudo-crossvanograms used less than half the data; thus potentially it could reduce more than half the sampling cost than kriging estimation. Cokriging with pseudo-crossvariograms was shown to be a precise and an economic way for determining nonpoint source pollutant distributions in large fields.

J. Environ. Qual. 28:424-428, 1999.

#### VACUUM METHOD FOR FIELD INSTALLATION OF PIPES AND CASINGS IN SANDY SOILS

#### L. Ulery, S. Stewart, D.A. Reid and P.J. Shouse

Soil moisture-monitoring equipment is difficult to install in poorly consolidated sand or sediments using hand tools because the loose material tends to collapse. The technique described herein uses a 5.5-hp wet/dry vacuum cleaner, powered by a portable gasoline generator, to remove the soil while an operator pushes a conductor pipe or casing into the profile. After initiating the hole using a hand bucket auger, an open-ended metal pipe or polyvinyl chloride (PVC) casing is inserted vertically into the shallow hole. A smaller tube, or stinger, attached to a wet/dry vacuum is inserted into the pipe to extract loose material while downward pressure is applied on the pipe. Once the casing is installed, instrumentation such as lysimeters, gypsum blocks, or tensiometers can be placed at the desired depth and backfilled with native soil. The casing is then raised and the soil allowed to collapse around the equipment, or the pipe can be left in place for neutron probe access. Measurements of soil water content after an infiltration experiment demonstrated uniform downward movement with minimal preferential flow or soil disturbance as a result of the vacuum installation of gypsum blocks and a neutron access tube.

Soil Sci.165:269-273, 2000.

# SPATIAL DEPENDENCE OF SOIL WATER RETENTION AND THERMAL PROPERTIES OF A SANDY LOAM SOIL

#### P.J. Shouse, B.P. Mohanty and T.H. Skaggs

Energy exchanges at the soil surface are propagated into the soil profile by a complex series of transport processes with rates affected by soil properties varying in both space and time. Our project focuses on the variation of volumetric heat capacity, thermal conductivity, and thermal diffusivity as functions of space and soil water retention. We measured the thermal properties of a sandy loam soil using the dual heat probe method on undisturbed soil cores equilibrated to different soil water pressure heads. The measured thermal properties depend on the water content and to a lesser extent the bulk density. Both thermal and retention properties varied in space as well.

Agronomy Abstract p. 193, 1999.

### NONLINEAR DYNAMICS OF SOIL MOISTURE AND TEMPERATURE AT DIFFERENT SCALES

#### P.J. Shouse, T.H. Skaggs and B.P. Mohanty

Dynamics of soil moisture and temperature at different spatio-temporal scales is critical for land-atmosphere interaction. We used gridded ground-based impedance probe water content data and aircraft-mounted Electronically Scanned Thinned Array Radiometer (ESTAR) pixel-average soil moisture data to investigate the spatio-temporal evolution and time-stable characteristics of soil moisture in three selected footprints from the Southern Great Plains 1997 (SGP97) Hydrology Experiment in Oklahoma. Better time stable features were observed within a footprint containing sandy loam soil than within two pixels containing silty loam soil. Additionally, flat topography with split wheat/grass land cover produced the largest spatio-temporal variability and the least time stability in soil moisture patterns. A comparison of ground-based and remote sensing data showed that ESTAR footprint-average soil moisture was well calibrated for the pixel with sandy loam soil, rolling topography, and pasture land cover, but improved calibration is warranted for the silty loam soil, rolling topography, pasture land and silty loam soil, flat topography, split vegetation of wheat and grass land with tillage practice pixels. Results from another field-scale soil moisture and temperature dynamics experiment in a sandy loam soil, flat topography, bare land cover, and semi-arid climate of Riverside, California will also be presented.

Agronomy Abstract p. 218, 2000.

# APPLICATION OF MOMENT ANALYSIS FOR ESTIMATING TRANSPORT AND REACTION PARAMETERS FROM BREAKTHROUGH CURVES

B.S. Das, I.W. Wraith, H.W. Langner, P.J. Shouse and G.J. Kluitenberg

The method of moments (MOM) was critically examined for estimating solute transport parameters and analyzing transport processes. Parameters were estimated from both laboratory- and field-measured breakthrough curves using the MOM and the conventional least-squares method. Results show that these two procedures yield similar estimates when a complete mass recovery is obtained. In cases of incomplete mass recovery, parameters associated with higher-order moments depart significantly from those estimated using least-squares methods. This suggests that where the MOM is indispensable, a complete mass balance should be ensured during the experimentation. Results of process analysis show that nonequilibrium indices, defined with moments, reveal interactions among transport and reaction processes. However, it is not possible to quantify these interactions unless extreme bounds for the indices are properly defined.

Agronomy Abstract p. 219, 2000.

### INVERSE OPTIMIZATION, CALIBRATION AND VALIDATION OF SIMULATION MODELS AT THE FIELD SCALE

#### J. Šimůnek and J.A. de Vos

An overview is given of the issues of parameter estimation, model verification, and model validation as applied to field-scale subsurface flow and transport problems. We briefly review inverse optimization methods for estimating soil hydraulic parameters from a variety of field experiments, including tension disc infiltrometry, cone penetrometry, and gravity drainage experiments. An example is presented showing calibration of the numerical HYDRUS-2D model using data of a tile-drainage experiment. The hydraulic characteristics of the layered soil profile at the site were identified based on the joined use of laboratory data, field monitoring data, and the numerical model. A split sampling technique was used to test applicability of the numerical model for this study.

*In:* J. Feyen and K. Wiyo (eds.), *Modelling of Transport Process in Soils at Various Scales in Time and Space*, pp. 431-445, Wageningen Pers, Wageningen, The Netherlands, 1999.

# HORIZONTAL INFILTRATION REVISITED USING PARAMETER ESTIMATION J. Šimůnek, J.W. Hopmans, D.R. Nielsen and M. Th. van Genuchten

A parameter estimation approach (the HYDRUS-1D model) was used to analyze horizontal infiltration data for Columbia silt loam and Hesperia sandy loam, presented and investigated previously by Nielsen et al. (1962) using the analytical method of Bruce and Klute (1956). Similarly to the original analysis, water content profiles at the different times could be accurately optimized in a simultaneous fashion only when the applied pressure head was close to saturation (-2 cm). For much lower boundary pressures (-50 and -100 cm), water content profiles for the different times had to be optimized independently. Excellent agreement was obtained between diffusivities calculated either analytically or numerically from the same water content profiles. In addition to diffusivities, the numerical parameter estimation analysis of the horizontal infiltration experiments provided estimates of the soil-water retention and hydraulic conductivity functions.

Am. Geophys. Union, p. 363, 1999.

### ESTIMATING HYSTERESIS IN THE SOIL WATER RETENTION FUNCTION FROM CONE PERMEAMETER EXPERIMENTS

### J. Šimůnek, R. Kodesova, M.M. Gribb and M. Th. van Genuchten

Data obtained from modified cone penetrometer experiments were used to estimate the hysteretic soil hydraulic properties with a parameter estimation technique which combined a numerical -solution of the Richards equation with Marquardt-Levenberg optimization. The modified cone penetrometer was designed to inject water into a soil through a cylindrical screen, measure the infiltration rate with time, and track the movement of the wetting front using two tensiometer rings positioned above the screen. After reaching relatively stable tensiometer readings during the experiments, the source of water was cut off and pressure head readings measured while water in the soil profile redistributed. Cumulative inflow and pressure head readings for two experiments with different supply pressures were analyzed to obtain estimates of the soil water retention and hydraulic conductivity functions. Analysis of flow responses obtained during the infiltration period, and of those obtained during the combined infiltration and redistribution phases, demonstrated the importance of hysteresis of the soil hydraulic functions. We found that the redistribution phase could not be described accurately when hysteresis was neglected. Hysteresis in the soil hydraulic functions was modeled using a relatively simple empirical model in which wetting scanning curves are scaled from the main wetting curve and drying scanning curves are scaled from the main drying curve. This model was deemed adequate for our examples. Optimization results for various combinations of unknown soil hydraulic parameters were compared to results of standard laboratory and in situ methods. Estimates of the saturated hydraulic conductivity were well within the range of in situ measurements. The estimated main hysteretic loops of the soil water retention curve were for the most part situated between the wetting and drying curves obtained with standard methods.

Water Resour. Res. 35(5):1329-1345, 1999.

# USING THE HYDRUS-1D AND HYDRUS-2D CODES FOR ESTIMATING UNSATURATED SOIL SOLUTE TRANSPORT PARAMETERS

### J. Šimůnek, M. Th. van Genuchten and M. Sejna

In this paper we describe a parameter estimation procedure which combines the Levenberg-Marquardt nonlinear parameter optimization method involving weighted least squares with either a one-dimensional numerical model (HYDRUS-1D) or a two- or quasi three-dimensional model (HYDRUS-2D), which solve the governing equations for water flow and solute transport in variably-saturated porous media. The procedure permits several unknown parameters in the unsaturated soil-hydraulic functions to be estimated from observed water contents, pressure heads, and/or instantaneous or cumulative boundary fluxes (e.g., infiltration or outflow data) during transient water flow by numerical inversion of the Richards equation. Additional retention or hydraulic conductivity data, as well as a penalty function for constraining the optimized parameters to remain in some feasible region (Bayesian estimation) can be optionally included in the parameter estimation procedure. Similarly, the procedure permits solute transport and/or reaction parameters to be estimated from observed concentrations and/or instantaneous or cumulative boundary solute fluxes during transient solute transport by numerical inversion of the convection-dispersion equation. The unsaturated soil hydraulic and solute transport and reaction parameters can be estimated either sequentially or simultaneously. Depending upon the quality of observed data, soil hydraulic or solute transport parameters for several soil layers can be estimated simultaneously. The parameter estimation procedure is demonstrated for several laboratory and field experiments.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, Part 1, pp. 1523-1536, University of California, Riverside, CA, 1999.

# THE HYDRUS-2D SOFTWARE PACKAGE FOR SIMULATING TWO-DIMENSIONAL MOVEMENT OF WATER, HEAT, AND MULTIPLE SOLUTES IN VARIABLY-SATURATED MEDIA, VERSION 2.0

### J. Šimůnek, M. Sejna and M. Th. van Genuchten

This report documents version 2.0 of HYDRUS-2D, a software package for simulating water, heat, and solute movement in two-dimensional variably saturated media. The software package consists of the HYDRUS2 computer program, and the interactive graphics-based user interface HYDRUS2D. The HYDRUS-2D program numerically solves the Richards' equation for saturated-unsaturated water flow and the convection-dispersion equation for heat and solute transport. The flow equation incorporates a sink term to account for water uptake by plant roots. The heat transport equation considers transport due to conduction and convection with flowing water. The solute transport equations consider convective-dispersive transport in the liquid phase, as well as diffusion in the gaseous phase. The transport equations also include provisions for nonlinear nonequilibrium reactions between the solid and liquid phases, linear equilibrium reactions between the liquid and gaseous phases, zero-order production, and two first-order degradation reactions: one which is independent of other solutes, and one which provides the coupling between solutes involved in sequential first-order decay reactions. In addition, physical nonequilibrium solute transport can be accounted for by assuming a two-region, dual-porosity type formulation which partitions the liquid phase into mobile and immobile regions. This version 2.0 of HYDRUS-2D also includes a Marquardt-Levenberg type parameter optimization algorithm for inverse estimation of soil hydraulic and/or solute transport and reaction parameters from measured transient or steady-state flow and/or transport data.

The program is distributed by means of two different options. Option A pertains to the executable HYDRUS2 code (a modification of the former CHAIN-2D code) for use with a graphics-based user interface, HYDRUS2D, for easy data preparation and output display in the MS Windows environment. This option also includes the HYDRUS2D interface, and a structured mesh generator for relatively simple flow domain geometries. Option B additionally includes a CAD program for more general domain geometries, and the MESHGEN2D mesh generator for an unstructured finite element mesh specifically designed for variably-saturated subsurface flow transport problems. This report serves as both a user manual and reference document. Detailed instructions are given for data input preparation.

IGWMC-7PS-53, Int. Ground Water Modeling Center, Colorado School of Mines Golden, CO. 251 p., 1999.

# INVERSE ANALYSIS OF TRANSIENT VARIABLY-SATURATED WATER FLOW AND SOLUTE TRANSPORT COLUMN STUDIES

### J. Šimůnek, J. Vanderborght and M. Th. van Genuchten

Two transient water flow and solute transport column experiments were studied using an inverse analysis. Large undisturbed soil columns (0.3-m i.d., 1-m long, 4 major soil horizons) were subjected to a periodic upper boundary con( involving a constant flow rate followed by a no-flow condition, with a period of 1 day. The lower boundary condition was either a constant pressure head I cm below a ceramic plate) or a seepage face (no ceramic plate). The soil was characterized as a sandy loam with a highly degraded illuvial day hot Water contents and solute concentrations were measured at 13 locations horizontally installed TDR probes. We first calibrated the water flow model against the water content measurements. The measured information was not deemed sufficient to estimate the true soil hydraulic parameters. Because resistances against water flow caused by the low-conductivity ceramic I great difficulties were encountered in calibrating the flow model using data for the constant lower boundary condition. Calibrated water flow fields measured concentrations were subsequently used to estimate dispersivities of particular soil horizons. Breakthrough curves at particular locations analyzed both sequentially and simultaneously. Results of the inverse analysis were compared with results of a quasi steady-state solution.

Geophysical Research Abstracts, European Geophysical Society 1(2):311, 1999.

# ESTIMATING UNSATURATED SOIL HYDRAULIC PROPERTIES FROM LABORATORY TENSION DISC INFILTROMETER EXPERIMENTS

#### J. Šimůnek, O. Wendroth and M. Th. van Genuchten

Four tension disc infiltration experiments were carried out on a loamy soil in the laboratory for the purpose of estimating the unsaturated soil hydraulic properties. Sixteen tensiometers were installed in pairs at the following coordinate (r, z) positions: (10, 2.5), (10, 5), (10, 10), (15, 5), (15, 10), (15, 15), (15, 15)20), and (15, 30), where y represents the distance from the axis of symmetry and z is the location below the soil surface. A time domain reflectometry (TDR) probe was used to measure water contents at a depth of 2 cm directly below the tension disc. The first three experiments involved supply pressure heads at the disc of -20, -10, -;5, and -1 cm, with the experiment lasting for approximately 5 hours. The same supply pressure heads were also used for the fourth experiment, which lasted 6.25 days so as to reach steady state at each applied tension. The measured data were analyzed using Wooding's [1968] analytical solution and by numerical inversion. The parameter estimation method combined a quasi three-dimensional numerical solution of the Richards equation with the Marquardt-Levenberg optimization scheme. The objective function for the parameter estimation analysis was defined using different combinations of the cumulative infiltrated volume, TDR readings, and tensiometer measurements. The estimated hydraulic properties were compared against results obtained with an evaporation experiment as analyzed with Wind's [1968] method. Water contents in the retention curves were underestimated when both transient and quasi steadystate experiments were analyzed by parameter estimation. Unsaturated hydraulic conductivities obtained by parameter estimation and using Wooding's [1968] analysis corresponded well. Drying branches of the hydraulic conductivity function determined by parameter estimation also corresponded well with those obtained with the evaporation method.

Water Resour. Res. 35(10):2965-2979, 1999.

# SOIL HYDRAULIC PROPERTIES FROM LABORATORY EVAPORATION EXPERIMENTS BY PARAMETER ESTIMATION

#### J. Šimůnek, O. Wendroth and M. Th. van Genuchten

We estimated the soil hydraulic properties from laboratory evaporation experiments using a parameter estimation method and the modified method of Wind [1968]. We used both numerically generated data and data measured in the laboratory. Two experiments with two different soils were performed in the laboratory. Both numerical and laboratory experiments were carried out on 10-cm high soil cores. Pressure heads inside the cores were measured with tensiometers at five different depths. While evaporative water loss from the top was determined by weighing the soil samples in the laboratory, a constant evaporation rate was specified for numerical experiments. The objective function for the parameter estimation analysis was defined in terms of the final total water volume in the core and pressure head readings of one or several tensiometers. An analysis of numerically generated data showed that the optimization method was most sensitive to the hydraulic parameters n and  $\theta_s$  and least to  $\theta_r$  ( $\theta_s$  is the saturated water content,  $\theta_n$  is the residual water content, and n is a hydraulic property shape factor). Numerical analysis also showed a very high correlation between parameters  $\theta_r$  and n. Pressure heads measured close to the soil surface were found to be more valuable for the parameter estimation technique than those measured at greater depths. The optimized hydraulic parameters for the laboratory soil samples corresponded closely with those obtained using Wind's analysis. All optimizations gave similar results for the soil hydraulic properties within the measurement range of the soil water pressure head (0 to -700 cm). Extrapolation beyond this range yielded a high level of uncertainty.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, Part 1, pp. 713-724, University of California, Riverside, CA, 1999.

# ESTIMATING HYSTERESIS IN THE SOIL WATER RETENTION FUNCTION FROM A COMBINED UPWARD INFILTRATION AND EVAPORATION EXPERIMENT

### J. Šimůnek, O. Wendroth, N. Wypler and M. Th. van Genuchten

Data obtained from an upward infiltration experiment followed by evaporation were used to estimate the hysteretic soil hydraulic properties. The invoked parameter estimation technique combined a numerical solution (HYDRUS-1D) of the Richards equation with Marquardt-Levenberg optimization. The laboratory experiments were carried out on 10-cm long soil cores having an internal diameter of 10 cm. A constant pressure head of 10 cm was used as the lower boundary condition for the upward infiltration experiment. A two-rate evaporation approach was followed for the evaporative water loss from the top was determined by weighing the soil samples. The objective function for the parameter estimation analysis was defined in terms of pressure head readings and the cumulative infiltration rate during upward infiltration and the final total water volume in the core as well as pressure head readings during the evaporation part. Analysis of flow responses obtained during the combined infiltration and evaporation phases demonstrated the importance of hysteresis of the soil hydraulic functions. We found that the evaporation phase could not be described accurately when hysteresis was neglected. The optimized hydraulic parameters were compared against those obtained using Wind's analysis.

Geophysical Research Abstracts, 1(2), European Geophysical Society: 305, 1999.

#### REVIEW OF INVERSE ESTIMATION OF SOIL HYDRAULIC PROPERTIES

### J.W. Hopmans and J. Šimůnek

Parameter estimation of flow and transport properties using numerical modeling of transient flow and transport experiments in combination with an optimization code has been applied only to a limited extend, principally for the estimation of soil hydraulic functions. The parameter estimation method is attractive since it applies to transient experiments and is therefore not constraint to assumptions of analytical solutions. Experiments could be designed to be simple and short, relative to methods that require static or near-equilibrium conditions. Although the inverse technique has been successfully applied by many, others have hesitated to investigate this method, because of lack of information or guidelines with regard to experimental setup, type, error and frequency of measurements, choice of optimization code, and unfamiliarity with technical jargon. Consequently, parameter estimation using transient experiments has been studied only to a limited extend. In many cases, questions arise with regard to which parameters to optimize, to the influence of errors associated with the optimized parameters, and which flow or transport variables to be included in the minimization function. A review of the inverse estimation of soil hydraulic characteristics will be presented.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, Part* 1, pp. 643-660, University of California, Riverside, CA, 1999.

# USING A MULTI-STEP SOIL -WATER EXTRACTION TECHNIQUE FOR IN-SITU ESTIMATION OF SOIL HYDRAULIC PROPERTIES

### M. Inoue, J. Šimůnek, J.W. Hopmans and V. Clausnitzer

Estimation of soil hydraulic properties is important to effectively provide input for transient water flow and solute transport simulations and predictions. The objective of this study was to demonstrate the potential application of in-situ soil water extraction to estimate soil water retention and unsaturated hydraulic conductivity parameters. The Levenberg-Marquardt algorithm in combination with the HYDRUS-2D flow code was used to inversely estimate the parameters of the hydraulic functions from transient soil matric potential and cumulative soil solution extraction measurements. An experiment was carried out in a field soil consisting of Yolo silt loam. A series of vacuum extraction pressures was applied to a ceramic soil solution sampler, and cumulative soil solution extraction volumes and matric potential heads at various locations near the extraction device were monitored during extraction. A power function determined from measured tensiometric data was used to calculate the matric potential at the lower boundary. The upper boundary was defined as a zero flux boundary. Cumulative extraction volume and matric potential data were included in an objective function that was minimized to estimate the parameters describing the hydraulic functions. We determined that the inverse solution was sensitive to the hydraulic resistance of the ceramic cylinder of the extraction device. The optimized parameters were correctly estimated after we included in the objective function three independently measured soil water retention data points determined during the extraction experiment. Comparison of the optimized soil hydraulic parameters with those determined independently with the instantaneous profile method indicated that the in-situ estimation using a multi-step soil-water extraction technique can provide accurate soil hydraulic data.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 725-736, University of California, Riverside, CA, 1999.

### ESTIMATION OF SOIL HYDRAULIC AND SOLUTE TRANSPORT PARAMETERS FROM TRANSIENT COLUMN EXPERIMENTS

#### M. Inoue, J. Šimůnek, S. Shiozawa and J.W. Hopmans

Estimation of soil hydraulic and solute transport parameters is important to provide input parameters for numerical models simulating transient water flow and solute transport. The Levenberg-Marquardt algorithm in combination with the HYDRUS-1 D (version 2.0) code was used to inversely estimate several unsaturated soil hydraulic and solute transport -parameters from transient pressure head, volumetric water content, and solute (NaCl) concentration measurements. A 30-cm long coarse-textured soil column having an internal diameter of 5 cm was used for the infiltration experiments. Experiments were carried out with both increasing and decreasing solute concentrations following sudden increases in the infiltration rate for the sand column. Pressure heads, volumetric water contents, and solute concentrations were measured using electric mini-tensiometers and four-electrode sensors. The optimization results were compared with independently measured soil water retention, unsaturated hydraulic conductivity, and solute dispersion data. The optimized values corresponded well with those measured independently within the range of experimental data.

Geophysical Research 1(2), European Geophysical Society, 311, 1999.

# NUMERICAL SIMULATION OF TRANSPORT AND SEQUENTIAL BIODEGRADATION OF CHLORINATED ALIPHATIC HYDROCARBONS USING CHAIN-2D

### D. Schaerlaekens, D. Mallants, J. Šimůnek and M. Th. van Genuchten

Microbiological degradation of perchloroethylene (PCE) under anaerobic conditions follows a series of chain reactions, in which, sequentially, trichloroethylene (TCE), cis-dichloroethylene (c-DCE), vinylchloride (VC) and ethene are generated. First-order degradation rate constants, partitioning coefficients and mass exchange rates for PCE, TCE, c-DCE and VC were compiled from the literature. The parameters were used in a case study of pump-and-treat remediation of a PCE-contaminated site near Tilburg, The Netherlands. Transport, non-equilibrium sorption and biodegradation chain processes at the site were simulated using the CHAIN-2D code without further calibration. The modelled PCE compared reasonably well with observed PCE concentrations in the pumped water. We also performed a scenario analysis by applying several increased reductive dechlorination rates, reflecting different degradation conditions (e.g., addition of yeast extract and citrate). The scenario analysis predicted considerably higher concentrations of the degradation products as a result of enhanced reductive dechlorination of PCE. The predicted levels of the very toxic compound VC were now an order of magnitude above the maximum permissible concentration levels.

Hydrol. Process 13:2847-2859, 1999.

### IDENTIFICATION OF THE HYDRAULIC CHARACTERISTICS OF A LAYERED SILT LOAM

### J.A. de Vos, J. Šimůnek, P.A.C. Raats and R.A. Feddes

The hydraulic characteristics of a layered silt loam were identified, based on the joint use of laboratory data, field monitoring data, and the two-dimensional Hydrus-2D model. Laboratory water retention and hydraulic conductivity characteristics and hydraulic conductivities at saturation were used in the Hydrus-2D model, with successive infiltration rates of 0.5, 1, 2, 3, 6, 10, 15, 20 and 25 mm d<sup>-1</sup>. The hydraulic conductivities at saturation for the different layers were optimised by comparing simulated (steady) and observed drain discharge rate - groundwater level relationships. Further adjustments were made on the basis of field-measured water retention characteristics for the 0-25 cm topsoil. It is shown that the hydraulic properties, in combination with a drain tile spacing of 12 m and typical weather patterns, lead to highly variable flow patterns. These varying flow patterns and momentary spatial distributions of the solutes explain the typical fluctuations of the solute concentration in the drainage water in relation to fluctuations in the drain discharge rate.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, Part* 1, pp. 783-798, University of California, Riverside, CA. 1999.

# SOIL HYDRAULIC PROPERTIES DETERMINED FROM EVAPORATION AND TENSION INFILTRATION EXPERIMENTS AND THEIR USE FOR MODELING FIELD MOISTURE STATUS

#### O. Wendroth and J. Šimůnek

Accurate determination of soil hydraulic properties over a wide range of moisture contents, especially close to water saturation still provides some difficulties. Moreover, the suitability of hydraulic properties determined under laboratory conditions for modeling field soil water status has to be proven. This study focuses on the correspondence between a modified Wind method and a steady-state disk permeameter infiltration method. Hydraulic properties determined in the laboratory were used for simulation of field soil water content time series, and the effect of a stochastic filter (Kalman Filter) on the prediction of soil water content with a state-space approach was evaluated. Results from both laboratory methods corresponded well. With a realistic estimate of field soil evaporation, lab-determined properties were suitable for simulation of field soil moisture status. While observations are taken into account in the state-space prediction, uncertainties due to e.g. an unrealistic high estimate of evaporation could be compensated.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 737-748, University of California, Riverside, CA, 1999.

# THE DISC COMPUTER SOFTWARE FOR ANALYZING TENSION DISC INFILTROMETER DATA BY PARAMETER ESTIMATION, VERSION 1.0

#### J. Šimůnek and M. Th. van Genuchten

This report documents version 1.0 of DISC, a computer software package for analyzing tension disc infiltrometer data by parameter estimation. The software package consists of the simplified HYDRUS2 computer program, and an interactive graphics-based user interface. The DISC code numerically solves the Richards' equation for saturated-unsaturated water flow. Flow occurs in a three-dimensional region exhibiting radial symmetry about the vertical axis. The software includes a Marquardt-Levenberg type parameter optimization algorithm for inverse estimation of soil hydraulic from measured transient cumulative infiltration and related data.

The governing flow and transport equations are solved numerically using Galerkin-type linear finite element schemes. The transport region is discretized automatically by the software into triangular elements using pregenerated files that are scaled directly to the specified size of the tension disc radius.

This report serves as both a user manual and reference document. Detailed instructions are given for data input preparation.

Research Report No. 145, U.S. Salinity Laboratory, USDA, ARS, Riverside CA. 34 p, 2000.

# INVERSE ESTIMATION OF UNSATURATED SOIL HYDRAULIC AND SOLUTE TRANSPORT PARAMETERS USING THE HYDRUS-1D CODE

#### J. Šimůnek and M. Th. van Genuchten

A numerical code (HYDRUS-1D) was developed for identifying soil-hydraulic and solute transport parameters from unsaturated flow and transport data in a on dimensional porous media. The utility of the code was demonstrated using data typically obtained during multistep outflow experiment, horizontal infiltration followed by redistribution, and a column miscible displacement (breakthrough) study. Because of its generality (in terms of the definition of the objective function, the possible combination of different boundary and initial conditions, and options for considering multi-layered systems), HYDRUS-1D is an extremely useful tool for analyzing a broad range of steady-state and transient laboratory and in-situ field flow and transport experiments.

*In*: Brian B. Looney and Ronald W. Falta (eds.), *Vadose Zone Science and Technology Solutions*, vol. 2, pp. 815-827, Battelle Press, Columbus, OH, 2000.

# RETCML: INCORPORATING MAXIMUM-LIKELIHOOD ESTIMATION PRINCIPLES IN THE RETC SOIL HYDRAULIC PARAMETER ESTIMATION CODE

### K.J. Hollenbeck, J. Šimůnek and M. Th. van Genuchten

RETC is a public domain computer code for estimating parameters of the water retention curve and hydraulic conductivity functions of unsaturated soils. RETC was developed at the U. S. Salinity Laboratory and is now used world-wide with thousands of copies distributed. Evaluation of the final estimation results in the code has been improved to yield a new version, RETCML, based on maximum-likelihood theory for the special case of weighted least-squares estimators. This paper first explains the theory of maximum-likelihood and introduces the principles of model adequacy and parameter uncertainty on a formal basis. Next, this paper presents a user guide for the code. RETCML is also free and has been programmed to be almost fully compatible with the original RETC input files, thus making it easy to re-analyze previous data. The output of RETCML includes a thorough evaluation of estimation results.

Computer & Geosciences 26(3):319-327, 2000.

#### INFILTRATION OF WATER INTO SOIL WITH CRACKS

#### V. Novak, J. Šimůnek and M. Th. van Genuchten

This paper presents the physical basis of the FRACTURE submodel for simulating infiltration of precipitation/irrigation water into relatively dry, cracked, fine-textured soils. The FRACTURE submodel forms part of the HYDRUS-ET variably saturated flow/transport model. Infiltration into the soil matrix is formally divided into two components: (1) vertical infiltration through the soil surface; and (2) lateral infiltration via soil cracks. The first component is described and solved using the 1D Richards' equation. Excess water that does not infiltrate through the soil surface is either considered to be runoff if no soil cracks are present, or routed into soil cracks from where it may laterally infiltrate into the soil matrix. Horizontal infiltration from soil cracks into the soil matrix is calculated using the Green-Ampt approach and incorporated as a positive source/sink term in the Richards' equation describing flow in the matrix. In addition to the hydraulic properties of the soil matrix, the FRACTURE submodel requires parameters characterizing the soil cracks, notably the specific crack length per surface area, and the relationship between crack porosity, and the gravimetric soil water content. An example problem shows that infiltration from soil cracks can be an important process affecting the soil water regime of cracked soils. A comparison with the more traditional approach involving surface infiltration only, indicates important differences in the soil water content distribution during a rainfall/irrigation event. This extension of the classical approach to include crack infiltration significantly improves the identification and prediction of the soil water regime.

J. Irrig. & Drain. Engrg. 126(1):41-47, 2000.

### NONEQUILIBRIUM WATER FLOW CHARACTERIZED FROM AN UPWARD INFILTRATION EXPERIMENT

### J. Šimůnek, O. Wendroth, N. Wypler and M.Th. van Genuchten

Data obtained from upward tension infiltration experiments were analyzed using the single-porosity Richards equation, as well as variably-saturated dual porosity and dual-permeability models characterizing nonequilibrium water flow. The laboratory experiments were carried out on 10-cm long soil cores having an internal diameter of 10 cm. Constant pressure heads of -10 and -1 cm were used as the lower boundary condition for the upward infiltration experiment. Each infiltration was followed by a one-rate evaporation experiment to reestablish initial conditions and to obtain the drying soil hydraulic properties. Pressure heads inside the cores were measured using five tensiometers, while evaporative water loss from the top was determined by weighing the soil samples. The data were analyzed using a parameter estimation technique that combined a numerical solution (the modified HYDRUS-1D) of the governing flow equation with Marquardt-Levenberg optimization. Analysis of flow responses obtained during the infiltration experiment demonstrated significant nonequilibrium flow behavior. This behavior could be well characterized using a two-region physical nonequilibrium model that divides the medium into inter- and intra-aggregate pores with first-order transfer of water between the two systems.

Geophysical Research Abstracts, European Geophysical Society p. 215, 2000.

### THE HYDRUS-1D AND HYDRUS-2D CODES FOR ESTIMATING UNSATURATED SOIL HYDRAULIC AND SOLUTE TRANSPORT PARAMETERS

#### J. Šimůnek, M. Sejna and M. Th. van Genuchten

We present new versions of the HYDRUS-1D and -2D software packages and demonstrate their use for estimating soil hydraulic and solute transport parameters. Both models can be calibrated for water flow and solute transport in single- or multi-layered systems. Pressure head, water content, and/or concentrations at several locations, fluxes across boundaries, and independently measured retention and/or hydraulic conductivity data, can be include in the objective function. We present applications of HYDRUS-1D for estimating soil hydraulic and transport parameters from one- and multi-step outflow experiments, evaporation experiments, upward infiltration, horizontal infiltration followed by redistribution, and column breakthrough curves. Applications of HYDRUS-2D are presented for data obtained using a multistep soilwater extraction technique, a modified cone penetrometer, and a tension disc infiltrometer.

Agronomy Abstract p. 357, 1999.

# THE STANMOD COMPUTER SOFTWARE FOR EVALUATING SOLUTE TRANSPORT IN POROUS MEDIA USING ANALYTICAL SOLUTIONS OF THE CONVECTION-DISPERSION EQUATION

J. Šimůnek, M. Th. van Genuchten, M. Sejna, N. Toride and F.J. Leij

A large number of computer programs now exists for evaluating solute transport in porous media using analytical solutions of the convection-dispersion equation. The purpose of this project was to integrate the most widely used models into one software package. STANMOD (STudio of ANalytical MODels) is a Windows based computer software package for evaluating solute transport in porous media using analytical solutions of the convection-dispersion solute transport equation. STANMOD includes the following models for one-dimensional transport problems: CXTFIT 2.0 (Toride et al., 1995), CFITM (van Genuchten, 1980), CFITIM (van Genuchten, 1981), and CHAIN (van Genuchten, 1985). STANMOD also includes the models 3DADE (Leij and Bradford, 1994) and N3DADE (Leij and Toride, 1997) for two-and three- dimensional transport problems. The graphics-based user-interface of STANMOD is largely based on libraries developed for the HYDRUS- 1D and HYDRUS-2D) software packages. We present several illustrative examples of breakthrough curve analyses.

Agronomy Abstract p. 418, 2000.

### LOCALIZED GROUND WATER RECHARGE THROUGH PIPES IN CALCIC HORIZONS

#### G. Rodriguez-Marin, J. Šimůnek, I.B. Harrison and J.M. Hendrickx

Small and large pipes have been observed in many indurated calcic horizons in New Mexico. A survey on the La Mesa surface in southern New Mexico along a 30 km long trench revealed that the area occupied by pipes varied from 15 to 19 percent. Therefore, we hypothesize that pipes play an important role for localized ground water recharge. We will present field measurements and simulations with the model HYDRUS-2D) to test this hypothesis.

Agronomy Abstract p. 217, 2000.

# CRITICAL PATH ANALYSIS OF PORE-SCALE NETWORK MODELS: POWER LAW LOCAL CONDUCTIVITIES AND FINITE-SIZED SYSTEMS

#### T.H. Skaggs and A.G. Hunt

Network models of randomly sized capillary tubes are commonly used as surrogate media in theoretical investigations of the transport properties of soils and rocks. The conductivity of network models can be calculated by critical path analysis (CPA), a method based on the connectivity of highly conducting pathways and the statistics of percolation theory. It is well established that CPA accurately calculates the steady-state conductivity of infinitely sized networks when: (1) local conductivities are spatially uncorrelated, (2) local conductivities are broadly distributed (spanning at least four orders-of-magnitude), and (3) local conductivities are exponential functions of random variables (e.g. capillary tube radii). Recently, Hunt (1998) used cluster statistics to show that the CPA conductivity can be corrected for finitesized systems, and derived a probabilistic relationship in which the expected system conductivity decreases with increasing system size (this result requires that the local conductivity distribution be independent of system size). We will show that there are subtleties involved in the application of CPA when the local conductivity is a power law function of random variables rather than an exponential function, as is the case when local flow is according to Poiseuille's Law. When there is a power law dependence, the distance between critical bonds diminishes to point where percolation statistic no longer apply, and conductance occurs on non-tortuous pathways that are nothing like those obtained for an exponential dependence. Additionally, we will show that the conductivity can be an increasing function of system size when the local conductivity distribution has a system-size dependent maximum. The analytical CPA results will be compared with numerical network calculations.

Am. Geophys. Union, p. 441, 1999.

#### PREDICTING SOIL PARTICLE-SIZE DISTRIBUTIONS FROM TEXTURE DATA

### T.H. Skaggs, P.J. Shouse, L.M. Arya and B.P. Mohanty

Previously, methods have been developed for predicting the soil-water retention curve from the more easily measured particle-size distribution (PSD). Often, however, it is necessary to estimate retention properties when only soil texture data are available (percent sand, silt, and clay), rather than the full PSD. We conducted a study to determine if it is possible to predict the PSD from soil texture data. Procedures were developed for relating texture data to parameter values in several candidate models of the PSD. The estimation methods were tested on approximately 100 soils from the SGP97 and UNSODA databases. The results were mixed, with some of the predicted PSDs being very accurate, while others were somewhat poor. Ongoing efforts are aimed at refining the methods and identifying the conditions under which accurate predictions can be expected.

Agronomy Abstract p. 191, 1999.

### A PROBABILISTIC RELATIONSHIP BETWEEN THE HYDRAULIC AND ELECTRICAL CONDUCTIVITIES AS A FUNCTION OF SCALE

### G. Hunt and T.H. Skaggs

Recent work using critical path analysis has indicated a simple relationship between the hydraulic, g<sup>h</sup>, and electrical, g<sup>e</sup>, conductivities of heterogeneous porous media. In that work, ionic concentration was treated as being uniform and the application of critical path analysis required the system size be infinite. We consider the effects of variability in ionic concentration and finite-size scaling, and use cluster statistics of percolation theory to determine a probabilistic relationship between g<sup>e</sup> and g<sup>h</sup>. We also clarify some aspects of the application of percolation theory and critical path analysis to saturated soils when local conductances are power laws of the radii of connecting pores. Conduction is shown to take place along paths that are not tortuous (in the sense of percolation theory).

Agronomy Abstract p. 191, 1999.

### SOIL WATER AND SALINITY USING TDR DURING CYCLIC WETTING AND DRYING

### T.H. Skaggs, P.J. Shouse and P. Castiglione

Time-domain reflectometry (TDR) is a potentially useful tool for monitoring water content and soil salinity in the irrigated west. Calibrating the TDR for meaningful salinity measurements can be difficult. We set up several experiments to help us determine the proper calibration for conditions of non-steady non-uniform water contents; one using cyclic irrigation and evaporation, and one using drainage from saturation with no evaporation. Our results indicate that a linear calibration model may be more appropriate for calculating the electrical conductivity of soil water (ECsw) or the electrical conductivity of the saturated soil paste extract (ECe). Further experiments are planned and results will be reported.

Agronomy Abstract p. 27, 2000.

#### SOIL PHYSICAL PROCESSES FROM THE PORE TO THE PEDON

#### M. Th. van Genuchten

The past several decades has seen tremendous progress in the conceptual understanding and mathematical description of vadose zone flow and transport processes. A large number of analytical and numerical models of varying degrees of complexity and dimensionality are now available to predict water flow and solute transport in variably-saturated porous media. The purpose of this presentation was to highlight recent progress in flow/transport research at especially the local (pedon) scale. Improved process-based understanding of underlying processes, continued advances in numerical methods development, and the presence of increasingly powerful computers, are now making it possible to couple the most important flow/transport processes and soil/rock properties relevant to a particular problem. Examples involve multicomponent major ion chemical transport, simulations of the soil-plant-atmosphere continuum, and multiphase flow. Special attention is focused on the problem of preferential flow in variably-saturated structured (fractured or macroporous) media, and the need for more user-friendly software to enable a more effective application of models to a variety of flow/transport problems in research and management. Also discussed is a recently developed hierarchical neural-network approach for improved estimation of the unsaturated soil hydraulic properties, and their uncertainty, from more readily available or more easily measured data.

*In*: A. Gardenas (ed.), Workshop Proc. "Scale and Variability Issues in the Soil-Hydrological System", p. 10. Swedish University of Agricultural Sciences, Uppsala, Sweden, Aug. 25-27, 1999.

### CHARACTERIZATION AND MEASUREMENT OF THE HYDRAULIC PROPERTIES OF UNSATURATED POROUS MEDIA

### M. Th. van Genuchten, F.J. Leij and L. Wu

These Proceedings document 143 edited papers presented at the International Workshop "Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media," held in Riverside, California, October 22-24, 1997. The workshop was organized to review various aspects of water flow and solute transport in unsaturated porous media, particularly with respect to the characterization and measurement of the unsaturated hydraulic properties (water retention, hydraulic conductivity). Knowledge of the hydraulic properties is indispensable for addressing many soil, hydrological, environmental, ecological and agricultural problems.

They are needed in nearly all basic and applied aspects of soil, water, nutrient, and salinity management research (including precision agriculture), and serve as integrated indices for soil quality. They are also needed in models for heat and mass transport near the soil surface to simulate the extent and effects of regional and global climate change, and to interpret or improve the utility of remotely sensed soil moisture data at a variety of spatial scales.

About 220 scientists and engineers from some 20 countries participated in the Workshop; they included soil physicists, hydrologists, chemical and petroleum engineers, geologists, and agricultural engineers. Topics presented at the Workshop ranged from theoretical to application-oriented research, and from modeling to laboratory and field experimentation. The multidisciplinary nature of the Workshop provided unique opportunities for participants to interact with each other, to appreciate issues and opportunities in porous media modeling and characterization, and to discover commonalities and differences between the various disciplines.

*In:* M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media, Parts* 1 and 2, University of California, Riverside, CA, 1602 p., 1999.

#### MODELING FLOW AND TRANSPORT PROCESSES AT THE LOCAL SCALE

### M. Th. van Genuchten, M.G. Schaap, B.P. Mohanty, J. Šimůnek and F.J. Leij

Much progress has been made during the past several decades in attempts to more realistically simulate variably-saturated water flow and solute transport in the subsurface. A large number of conceptual models are now available to predict flow and transport in the vadose zone. In this paper we highlight recent advances in modeling at especially the local scale. Improved understanding of underlying processes, continued advances in numerical methods, and the introduction of increasingly powerful computers now permit comprehensive simulations of the most important physical, chemical and biological processes operative in the unsaturated zone.

Examples include models for mass/energy transport in the soil-plant atmosphere continuum, multicomponent major ion chemistry, and multifluid flow. While the problem of preferential flow remains a challenge, several useful approaches have recently become available to study and model preferential flow in structured media. Increasingly accurate indirect methods, including pedotransfer functions, are now also available for estimating the unsaturated soil hydraulic properties from more readily available or easily measured data. A need still exists for more user-friendly software to enable more effective application of models to a variety of flow and transport problems in research and management.

*In*: J. Feyen and K. Wiyo (eds.), *Modelling of Transport Process in Soils at Various Scales in Time and Space*, pp. 23-45, Wageningen Pers, Wageningen, The Netherlands, 1999.

#### RECENT ADVANCES IN VADOSE ZONE FLOW AND TRANSPORT MODELING

### M. Th. van Genuchten and E.A. Sudicky

The fate and transport of a variety of chemicals migrating from industrial and municipal waste disposal sites, or applied to. agricultural lands, is increasingly becoming a concern. Once released into the subsurface, these chemicals are subject to a large number of simultaneous physical, chemical, and biological processes, including sorption-desorption, volatilization, and degradation. Depending upon the type of organic chemical involved, transport may also be subject to multiphase flow that involves partitioning of the chemical between different fluid phases. Many models of varying degree of complexity and dimensionality have been developed during the past several decades to quantify the basic physicochemical processes affecting transport in the unsaturated zone. Models for variably saturated water flow, solute transport, aqueous chemistry, and cation exchange were initially developed mostly independently of each other, and only recently has there been a significant effort to couple the different processes involved. Also, most solute transport models in the past considered only one solute. For example, the processes of adsorption-desorption and cation exchange were often accounted for by using relatively simple linear or nonlinear Freundlich isotherms such that all reactions between the solid and liquid phases were forced to be lumped into a single distribution coefficient, and possibly a nonlinear exponent. Other processes such as precipitation-dissolution', biodegradation, volatilization, or radioactive decay were generally simulated by means of simple first- and/or zero-order rate processes. These simplifying approaches were needed to keep the mathematics relatively simple in view of the limitations of previously available computers. The problem of coupling models for water flow and solute transport with multicomponent chemical equilibrium and nonequilibrium models is now increasingly being addressed, facilitated by the introduction of more powerful computers, development of more advanced numerical techniques, and improved understanding of the underlying transport processes.

In this chapter we focus on alternative conceptual approaches for deterministic modeling of solute transport in variably saturated media. Among the topics discussed are single-ion equilibrium and nonequilibrium transport, sorption, degradation, volatilization, and multicomponent transport. Transport in 'Variably saturated structured systems is treated in somewhat more detail to illustrate the potential value of numerical models as useful tools for improving our understanding of the underlying transport processes at the field scale. We also briefly review recent developments in numerical techniques used for solving the governing flow and transport equations, including methods for solving large sparse matrices resulting from spatial and temporal numerical discretization .

*In*: M. B. Parlange and J. W. Hopmans (eds.). *Vadose Zone Hydrology., Cutting Across Disciplines*, pp. 155-193, Oxford University Press, New York, 1999.

#### SUFI: AN INVERSE PROGRAM FOR CONDITIONAL PARAMETER ESTIMATION

### K.C. Abbaspour, R. Schulin and M. Th. van Genuchten

SUFI (Sequential Uncertainty domain parameter Fitting) is a program that can be used for parameter fitting and parameter conditioning. Parameter fitting refers to a generic fitting objective where a certain function of unknown parameters is fitted to a set of measured data. Parameter conditioning refers to an objective where uncertain model input parameters are conditioned on measured model outputs. Contrary to fitting, in conditioning all measurements are respected by the probabilistic model of input parameters. In this paper the program SUFI is described and two examples are given to demonstrate the conditioning feature of SUFI. In the first example, simultaneous measurements of pressure head and water content are used to condition residual water content, saturated water content, and van Genuchten shape parameters  $\alpha$  and n. In the second example measured discharge is used to condition five parameters: residual water content, saturated water content, saturated hydraulic conductivity, and  $\alpha$  and n.

In: M. Th. van Genuchten, F. J. Leij and L.Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 705-712, University of California, Riverside, CA, 1999.

# SIGNIFICANCE OF MACROPOROSITY AND HYDROLOGY FOR SOIL MANAGEMENT AND SUSTAINABILITY OF AGRICULTURAL PRODUCTION IN A HUMID-TROPICAL ENVIRONMENT

L.M. Arya, T.S. Dierolf, A. Sofyan, P. Widjaja-Adhi and M. Th. van Genuchten

This paper analyzes soil-related agronomic constraints in the Sitiung region of Indonesia that are directly related to low nutrient-holding capacity, macroporosity, and rainfall regime. This region receives 2500 to 3000 mm of rainfall per year, but nearly 50% of the rainfall is disposed of rapidly via internal drainage. Although rapid internal drainage reduces the risks of erosion, it leads to infertility, acidity, and Al toxicity. The physical structure of the soils is characterized by stable aggregates, with numerous macropores in the surface and a predominantly microporous subsoil matrix interspersed with a few larger macropores. Macropores account for about 29% of porosity in the surface and between 3 and 6% in the subsoil. The saturated hydraulic conductivity of the matrix containing macropores averages about 300 to 400 cm/day, whereas that of the microporous matrix is generally <1 cm/day. The structure facilitates rapid infiltration and leaching of rainfall. However, little opportunity exists for nutrients moving downward with drainage water to accumulate in the subsoil. The main reason for this seems to be the low hydraulic conductivity and the preponderance of excessive wetness in the subsoil. Drying seems to be essential for movement of nutrients into the subsoil matrix. However, most of the agronomic crops are sensitive to Al toxicity and fail to grow roots deeper than 10 to 15 cm. Thus, they suffer from water stress, despite heavy and frequent rainfall, and fail to cause drying of the subsoil. Problems of acidity Al toxicity, and infertility worsen progressively where agricultural production consists mainly of Al-sensitive crops. Although liming with calcium carbonate improves the soil chemical environment, downward movement of lime is very slow. Deep liming is effective in improving rooting depth, crop water availability, and drying of the subsoil, but the technology is cost- and labor-intensive. Native vegetation, on the other hand, is able to grow roots to considerable depths and causes significant drying of the subsoil, even without soil amendments. Thus, production systems in which locally adapted vegetation of economic value is the main focus seem to be more sustainable and conducive to improving soil conditions.

Soil Science 164(8):586-601, 1999.

### MODELING NONWETTING PHASE PERMEABILITY USING ANALYTICAL AND NETWORK MODELS

#### U. Fischer, M.A. Celia, H. Fluhler and M. Th. van Genuchten

Nonwetting-phase relative permeabilities may be predicted from retention-curve data using a variety of analytical models as well as pore-scale network models. Analytical models that do not account for a discontinuous nonwetting phase fail to predict relative gas permeabilities, while models that account for this phenomenon result in very good predictions. Prediction of relative permeabilities with these analytical models requires stipulation of at least one additional parameter after fitting the retention curve. And these analytical models cannot predict absolute permeabilities without some permeability data. Comparisons of predicted gas permeabilities to measured data for two sandy soils indicate that the network model used provides good estimates of both relative and absolute permeabilities, and can accommodate a discontinuous gas phase, without any parameters beyond those needed to fit the retention curve. While the predicted magnitude of the hysteresis effect in the relative gas permeability functions was not large enough, the predictions obtained with the network model were much better than those calculated with the only analytical model that can be used for prediction of relative permeabilities on the basis of retention data only.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 145-154, University of California, Riverside, CA, 1999.

### GENERAL MODEL OF THE HYDRAULIC CONDUCTIVITY OF UNSATURATED SOILS

#### H. Hoffmann-Riem, M. Th. van Genuchten and H. Fluhler

A number of simple theoretical models are widely used to predict the unsaturated hydraulic conductivity of a soil. These models are based on the Hagen-Poiseuille equation, the Young-Laplace equation and several simplifying assumptions regarding the properties of the pore space. We propose a general model which is based on these assumptions but offers greater flexibility than the existing models. The models of Burdine, Mualem and others correspond to particular cases of this general model. A 'soil hydraulic index' is defined to compare the different models.

We then evaluate the validity of some common assumptions by applying different models to data sets taken from the UNSODA data base. To obtain a good fit, at least two parameters of the general model need to be optimized for each data set. In many cases, a reasonable fit requires parameter values that are not physically meaningful. We therefore believe that neither the general model nor the simpler models of Burdine and Mualem should be interpreted as physically-based models.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 31-42, University of California, Riverside, CA, 1999.

### DISTRIBUTION OF ECOLOGICALLY SIGNIFICANT FRACTIONS OF SELECTED HEAVY METALS IN THE SOIL PROFILE

### T. Nemeth, K. Bujtas, J. Csillag, G. Partay, A. Lukacs and M. Th. van Genuchten

The amount of wastes, wastewaters, and sewage sludges produced by agricultural, industrial, and municipal activities is rapidly increasing worldwide. In developing regions of the world this may be simply the result of an improving supply of clean tap water and canalization. Because of increasing environmental awareness, dumping of sewage into surface waters is subject to more strict regulations; thus, the amount of wastewaters subjected to treatments is also increasing in non-industrialized countries. Consequently, much growth in sewage sludge production may be expected, especially when taking into account the higher requirements and standards for wastewater treatment.

In Hungary approximately 1000 million cubic meters (m³) of wastewater were produced per year in the mid '80s, of which only 187 million m³ were sufficiently treated, the majority only partially treated, and 173 million m³ not treated at all. At that time, there was an increasing gap between the development of municipal water supply and of sewage systems, with the latter lagging behind the substantial improvements in water supply. The collection and proper treatment of liquid wastes is still a problem for many smaller municipalities. According to recent data, the amount of sewage in Hungary is above 1 million m³ per year. About 40% of these sludges are being deposited on agricultural fields and on forest plantations.

One reasonable and economic way to dispose of wastewaters and sludges is to apply them to agricultural fields, thereby exploiting their water and nutrient content. Currently, this practice is becoming increasingly important in many countries. In the early nineties about 30-50% of the sewage sludges were disposed by land application in the majority of the industrialized European countries, which compares to 33% of the annual sludge production in the United States.

*In: H. M.* Selim. and I. K. Iskandar (eds.). *Fate and Transport of Heavy Metals in the Vadose Zone*, pp. 251-271, Lewis Publ., Boca Raton, FL, 1999.

### TWO-MODEL SOIL WATER RETENTION AND FLOW MODEL NUMERICAL SIMULATION

#### H.A. Sobczuk and M. Th. van Genuchten

Local heterogeneity forces water to flow along complicated paths. Some of the flow paths are interconnected and allow water to flow through the soil system, but some of them are dead ended. The water in dead-end paths will flow until equilibrium of the potential between internal volume and the inlet of the flow path is reached. Any change in the water potential in the inlet will cause a change in the water amount within the volume of dead-end flow. We propose to distinguish two domains within the soil. One, called the mobile domain, takes part in the macroscopic water flow due to a global potential gradient (interconnected paths), and a second, the stagnant domain (containing dead- end pores) where water redistributes according to a local potential gradient.

The proposed model introduces a domain distinction in terms of flow ability. The distinction between both domains is connected with the water flow geometry rather then with the soil phase geometry itself, i.e., it is dependent on the flow intensity and /or direction. Results of numerical simulations in comparison to the Richards equation are presented.

Geophysical Research Abstracts, European Geophysical Society 1(2):328, 1999.

### THE IMPORTANCE OF JOHN R. PHILIP'S WORK TO MOTIVATING NUMERICAL ANALYSES OF VARIABLY-SATURATED FLOW

### M. Th. van Genuchten and J. Šimůnek

John R. Philip's formidable contributions to understanding and quantifying unsaturated flow and solute transport are too numerous to list. In our research they included his two- and multiple-term infiltration equations, his analytical solutions for horizontal and vertical unsaturated flow, studies of solute transport in aggregated media containing dead-end pores, heat transport in soils, and detailed analytical distributions of water flow around subsurface cavities. We show how several of his studies improved our own research during the past 25 years, especially the testing of numerical solutions of the Richards equation. While variably-saturated flow studies using increasingly sophisticated numerical techniques and more powerful computers have expanded well beyond the analytical applications of Philip's work, sometimes against his wish, they would have been impossible without his leadership and motivation. John Philip will long be remembered in the soil physics and vadose zone hydrology communities.

EOS Transactions Am. Geophys. Union 80(46):498, 2000.

### MEASUREMENT AND CHARACTERIZATION OF NONEQUILIBRIUM FLOW IN VARIABLY-SATURATED SOILS

### M. Th. van Genuchten, J. Šimůnek and O. Wendroth

Soil hydraulic properties are often measured in the laboratory using a variety of steady-state and transient drying methods (including evaporation and one- or multistep outflow methods). Before such experiments are initiated, samples are usually saturated with the goal of achieving full water saturation. Parameters obtained from such measurements are then often used in simulation models. to predict water flow in the near-surface environment. Unfortunately, very little attention is being paid to the fact that saturation levels measured in the laboratory are hardly ever achieved in the field, and that preferential flow typical of field wetting processes are seldom observed using experiments involving a drying process. In this paper we present evidence of nonequilibrium water flow during an upward laboratory infiltration experiment using an undisturbed structured (macroporous) 10-cm long soil sample. Each infiltration was followed by an evaporation experiment to re-establish initial conditions, and to obtain the drying curves. Measured infiltration rated and observed pressure heads within the sample reflect significant nonequilibrium flow associated with air entrapment within the aggregates (the soil matrix) and the presence of a complex flow pattern between the larger interaggregate pores and smaller intra-aggregate pores within the soil matrix. The nonequilibrium flow behavior could be well characterized using a two-region dual-permeability model. Implications of the observed data and invoked models are discussed relative to obtaining improved variably-saturated flow predictions in the field.

Int. Workshop and Tutorial Lectures on "Subsurface Flow and Transport Phenomena", Section for Hydrology and Ecology, Faculty of Civil Engineering & Geosciences, Delft Univ. of Technology, The Netherlands, October 23-27, 2000.

### UNSATURATED HYDRAULIC PROPERTY ESTIMATION IN SUPPORT OF SUBSURFACE FLOW AND TRANSPORT MODELING

#### M. Th. van Genuchten

The unsaturated soil hydraulic functions (the water retention and hydraulic conductivity curves) are critical parameters in many hydrologic, subsurface pollution and crop production studies. Current methods to directly measure these highly nonlinear properties are time-consuming and costly, and generally yield only approximate answers in view of the overwhelming heterogeneity of the subsurface. In this presentation we review several methods, including especially pedotransfer functions, for estimating the hydraulic properties from more easily measured data (notably soil texture and bulk density). A hierarchical neural network/bootstrap approach is used to obtain pedotransfer functions estimates of the unsaturated hydraulic functions, and their uncertainty, as a function of increased data availability. The often ignored effects of soil structure and macroporosity on the hydraulic properties, and indirectly on water flow and solute transport predictions, are also discussed. Dual-porosity type functions for the unsaturated hydraulic conductivity of structured media are shown to provide reasonable descriptions of preferential flow in several field experiments. Assuming the presence of immobile water further improved the transport predictions. The use of dual-porosity type hydraulic properties seems justified in view of many data sets which show that the measured saturated hydraulic conductivity is generally about an order of magnitude larger than the saturation end-point of the measured unsaturated hydraulic conductivity curve.

Fourth Int. Conf. on Environmetrics and Chemometrics, Las Vegas, NV, Sept. 18-20, 2000.

### EFFECT OF THE SHAPE OF THE SOIL HYDRAULIC FUNCTIONS NEAR SATURATION ON VARIABLY-SATURATED FLOW PREDICTIONS

### T. Vogel, M. Th. van Genuchten and M. Cislerova

Relatively small changes in the shape of the soil water retention curve near saturation can significantly affect the results of numerical simulations of variably saturated flow, including the performance of the numerical scheme itself in terms of stability and rate of convergence. In this paper, we use a modified form of the van Genuchten-Mualem (VGM) soil hydraulic functions to account for a very small, but non-zero minimum capillary height, h<sub>s</sub> in the soil water retention curve. The modified VGM model is contrasted with the original formulation by comparing simulation results for infiltration in homogeneous soils assuming both constant pressure and constant flux boundary conditions. The two models gave significantly different results for infiltration in fine-textured soils, even for h<sub>s</sub>-values as small as -1 cm. Incorporating a small minimum capillary height in the hydraulic properties leads to less non-linearity in the hydraulic conductivity function near saturation and, because of this, to more stable numerical solutions of the flow equation. This study indicates an urgent need for experimental studies that assess the precise shape of the hydraulic conductivity curve near saturation, especially for relatively fine-textured soils. For one example we found considerable improvement in the predicted conductivity function when a value of -2 cm for h<sub>s</sub> was used in the modified VGM model.

Adv. Water Resour. 24(2):133-144, 2000.

#### DYNAMICS OF WATER AND SOLUTE MOVEMENT IN AGGREGATED SOILS

### M. Th. van Genuchten, B. Mohanty and J. Šimůnek

Water flow and solute transport are generally considered equilibrium processes which assume that all parts of the liquid phase contribute equally to the flow or transport process. In reality, most field soils exhibit a variety of heterogeneities that cause deviations from equilibrium. Heterogeneity at relatively small scales is reflected by preferential flow through soil macropores and rock fractures. This paper reviews several approaches for modeling flow and transport in structured soils or unsaturated fractured rock. The approaches involve dual-porosity models that assume the presence of distinct mobile and immobile liquid phases in the flow domain, and dual-permeability models that assume that water can flow through both the fractures and soil matrix. Of particular importance in these models are the exchange terms governing water and chemical transfer between the macropores and micropores. Several applications of the two modeling approaches are discussed.

Agronomy Abstract p. 198-199, 1999.

# ATMOSPHERIC VOLATILIZATION OF METHYL BROMIDE, 1,3-DICHLOROPROPENE, AND PROPARGYL BROMIDE THROUGH TWO PLASTIC FILMS: TRANSFER COEFFICIENT AND TEMPERATURE EFFECT

### D. Wang, S.R. Yates, J. Gan and J.A. Knuteson

Atmospheric emission of methyl bromide (MeBr) and its potential alternative chemicals such as 1,3-dichloropropene (1,3-D) and propargyl bromide (PrBr) can contribute to air pollution and ozone depletion (for MeBr). One of the main sources of these chemicals is from agricultural soil fumigation. To understand the volatilization dynamics, emission of MeBr, 1,3-D, and PrBr through a polyethylene-based high-barrier film (HBF) and a virtually impermeable film (VIF) was measured using an air flow and sampling system that produced >90% mass balance. The experiment was conducted outdoors and was subjected to ambient daily temperature variations. The HBF film was found to be very permeable to 1,3-D and PrBr, but somewhat less permeable to MeBr. The VIF film was very impermeable to 1,3-D, PrBr, or MeBr. Measured volatilization flux, in general, exhibited strong diurnal variations which were controlled by film temperature. Unlike the HBF film, a time lag (~ 12 h) was observed between high-temperatures and high-emission flux values for the VIF film. An impermeable film may be used as an effective means of controlling the atmospheric emission of MeBr and its alternative chemicals.

Atmospheric Environment 33:401-407, 1999.

# SPATIAL AND TEMPORAL DISTRIBUTIONS OF 1,3-DICHLOROPROPENE IN SOIL UNDER DRIP AND SHANK APPLICATION AND IMPLICATIONS FOR PEST CONTROL EFFICACY USING CONCENTRATION-TIME INDEX

### D. Wang and S.R. Yates

A field experiment was conducted to study the spatial and temporal distributions of (EZ)1,3-dichloropropene (1,3-D) in the soil and effects on pest control efficacy. An emulsifiable concentrate formulation of 1,3-D (Telone EC) was applied with drip irrigation at 47kg AI ha<sup>-1</sup> to two different depths (2.5 and 20.3 cm, respectively). Comparisons were made between the two drip treatments and a direct shank injection of 1,3-D (Telone II) at 112kg AI ha<sup>-1</sup>. Concentrations of 1,3-D in soil air were measured at several locations over time to determine the spatial and temporal characteristics, and. to calculate the concentration-time index (CT). Citrus nematodes (Tylenchulus semipenetrans) were placed in the fumigated soil at 25 cm depth and their mortality rates were compared to the calculated CT. Distributions of 1,3-D were found to be relatively uniform in both the drip irrigation and the shank injection treatment. An application rate of 47kg ha<sup>-1</sup> with drip irrigation was sufficient to achieve significant concentration levels in soil beds. Applying 1,3-D with direct shank injection at 112 kg ha<sup>-1</sup> extended the measurable concentration levels to the furrows between the soil beds and to a depth of 1 m below the soil surface. Effective control of T. semipenetrans was achieved with both the drip irrigation and the shank injection. A threshold soil 1,3-D CT value of 12 µg h cm<sup>-1</sup> <sup>3</sup> was needed to reach a 100% efficacy for T. semipenetrans. The study indicates that 1,3-D fumigation may be carried out with drip irrigation at very low rate, and a CT index may be derived to aid in the determination of a minimum effective dosage.

Pesticide Science 55:154-160, 1999.

### AUTOMATED SEQUENTIAL SAMPLER FOR COLLECTION OF HIGHLY VOLATILE ATMOSPHERIC CONTAMINANTS

### D. Wang, F.F. Ernst and S.R. Yates

Rapid and accurate measurement of atmospheric concentrations of highly volatile organic compounds is important in obtaining reliable information for the assessment of environmental pollution or the volatilization mechanisms of the chemicals. Nonmechanized sample collection requires intensive labor and effort, and may cause large random or systematic errors. An automated solenoid switching system was developed to assist in obtaining precise environmental concentrations of highly volatile organic compounds. The design, construction, and operation are described in the paper for potential application in similar studies. Using this sampling system, two experiments were conducted to determine atmospheric volatilization flux density of three highly volatile and reactive organic compounds (methyl bromide, 1,3-dichloropropene, and propargyl bromide). The automated solenoid switching system significantly reduced the requirements for labor and time. Results from the two experiments indicate that reliable sample collection was achieved. The automated sampling system was also relatively inexpensive and can be easily modified to accommodate a variety of sources, sampling intervals, and multiple number of solenoid valves.

J. Environ. Qual. 28:345-349, 1999.

### ACCURACY OF SOIL HYDRAULIC PROPERTY ESTIMATION USING INFILTROMETERS HAVING DIFFERENT DISK SIZES

### D. Wang, S.R. Yates and M. Th. van Genuchten

Soil hydraulic properties, such as the saturated hydraulic conductivity  $(K_s)$  and the parameter ( $\alpha$ ) used in exponential expressions of the hydraulic conductivity function, are important in modeling water flow and solute transport in unsaturated soil profiles. Tension infiltrometers have become popular instruments for the determination of soil hydraulic properties under field conditions. However, estimated  $K_c$  and  $\alpha$  values using other independent field or laboratory measurements are often found to be different from those obtained with the infiltrometer method using approximate steady-state solutions. This is likely caused by the variable sizes of the infiltrometer disk used for the infiltration measurement and/or the limitations of steady-state solutions for small disk dimensions. To determine the effect of disk size on parameter estimation, we measured the infiltration in two soils (Arlington sandy loam and Sparta sand) with tension infiltrometers having several disk diameters (5.5-34.5 cm). For each disk size, the infiltration was repeated at multiple supply potentials, while measurements continued until steady-state, so that replicated parameter estimates were obtained. Results suggest that estimated values of  $(K_s)$  and  $\alpha$  appeared to vary with the size of the infiltrometer disk used. Variations in estimated  $(K_a)$  and  $\alpha$  values for different disk sizes, or for different potential increments for the same disk, were greater than the possible overestimation with the steady-state solution, as compared to an improved solution for small disk sizes. Discrepancies between tension infiltrometer and other methods in practice are caused probably more by variability within each method such as soil heterogeneity or simplification of the hydraulic conductivity function to an exponential expression, rather than by inherent limitations of the steadystate solutions.

In: M. Th. van Genuchten, F. J. Leij and L. Wu (eds.), Proc. Int. Workshop, *Characterization and Measurement of the Hydraulic Properties of Unsaturated Porous Media*, Part 1, pp. 563-570, University of California, Riverside, CA, 1999.

### TWO-DIMENSIONAL MODEL SIMULATION OF 1,3-DICHLOROPROPENE VOLATILIZATION AND TRANSPORT IN A FIELD SOIL

#### D. Wang, J.A. Knuteson and S.R. Yates

A modeling study was conducted to simulate 1,3-dichloropropene (1,3-D) emission and concentration distribution in soil profiles when the chemical was applied with subsurface drip irrigation with reduced rate. The purpose was to evaluate the effect on emission reduction as compared with conventional shank injection application. To compare with field measurements, simulated scenarios included a shallow drip application at 2.5 cm, covered with a polyethylene film; a deep drip application at 20.3 cm with bare soil surface; and a conventional shank injection at 30.5 cm with a regular application rate. A convective and diffusive two-dimensional model was used to simulate the simultaneous transport of 1,3-D in both liquid and gaseous phases. Diurnal variations of soil temperature were predicted to calculate 1,3-D diffusion coefficient and the Henry's constant. Predicted 1,3-D emissions compared well with field measurements for the shallow and deep drip irrigation treatments. The model simulation under-predicted 1,3-D emission in the shank injection plot, where other transport mechanisms such as gas phase convection likely occurred during and immediately after application. Results from the modeling study indicate that computer simulation can be used effectively to study the environmental fate and transport of 1,3-D under conditions where vapor phase diffusion and liquid phase convection are the dominant transport mechanisms. Applying 1,3-D with subsurface drip irrigation appeared to be useful for emission reduction.

J. Environ. Qual. 29:639-644, 2000.

### ATMOSPHERIC VOLATILIZATION OF 1,3-DICHLOROPROPENE UNDER DIFFERENT APPLICATION METHODS

#### D. Wang, S.R Yates, F.F. Ernst and J.A. Knuteson

A field experiment was conducted to study the effectiveness of 1,3-dichloropropene (1,3-D) application using subsurface drip irrigation with reduced dosage in decreasing atmospheric emission from soil fumigation. Comparison was made between a shallow drip application at 2.5 cm covered with a polyethylene film, a deep drip application at 20.3 cm with bare soil surface, and a conventional shank injection at 30.5 cm at a regular application rate. Atmospheric emissions of 1,3-D were continuously measured with seven replicated active chambers from the three treatments. Results indicated that total 1,3-D emission loss was over 90% in the shank injection, and 57% and 66% for the deep and shallow drip plots, respectively. The emission loss was extremely high in the shank injection plot since about 80% was emitted from the bed furrows where the slanted shanks left uncompacted fractures. On a per mass basis, the shank plot had 13.7 g lost per meter of field bed, whereas the deep and shallow drip plots had only 3.3 and 3.8 g of 1,3-D lost per meter length, respectively. This is a significant reduction in terms of total 1,3-D emission into the atmosphere. Applying 1,3-D using subsurface drip irrigation with reduced dosage has a great potential for emission reduction.

Water, Air & Soil Pollution 127(1/4):109-123, 2000.

### TRANSFORMATION AND DETOXIFICATION OF HALOGENATED FUMIGANTS BY AMMONIUM THIOSULFATE

### D. Wang, J. Gan, S.K. Papiernik and S.R. Yates

Fumigants are commonly used at high rates (100-400 kg ha¹) in warm regions to control soil-borne pests. Many fumigants, however, tend to move easily from the treated soil into the atmosphere or groundwater, resulting in air or groundwater pollution. We studied the transformation of the fumigants methyl bromide (MeBr), propargyl bromide (PBr), 1,3-dichloropropene (1,3-D), chloropicrin (CP), and methyl iodide (MeI) by fertilizer ammonium thiosulfate (ATS). All fumigants were rapidly dehalogenated by thiosulfate via nucleophilic substitution, and the rate of transformation followed the order MeBr  $\approx$  MeI > PBr > 1,3-D > CP. For all fumigants, the reaction followed second order kinetics with activation energy of  $\sim$ 73 KS mol¹, suggesting a similar rate-limiting step. In soil, amendment of ATS at 1.0 mmol kg¹ accelerated fumigant dissipation by 21-63 times for MeBr, MeI, and PBr and by 4.6-5.5 times for 1,3-D and CP. Preliminary toxicity assays using the luminescent bacterium *Vibrio fisheri* showed, that ATS transformation largely eliminated the acute toxicity of fumigants to this organism. These results suggest that thiosulfate transformation of halogenated fumigants is likely a benign chemical approach that may be used for mitigating environmental and health risks in fumigation.

Environ. Sci. Technol. 34:3717-3721, 2000.

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Environ. Sci. Technol. 34:3717-3721, 2000.

### METHODS FOR REMOVING AND DECOMPOSING METHYL BROMIDE FROM FUMIGATION GASES.

#### S.R. Yates and J. Gan

A method for the removal and rapid decomposition of halogenated fumigation agents is described. A fumigation agent, such as methyl bromide, contained in the gas stream exiting a fumigation chamber or structure is captured on activated carbon or other retentive substrate and rapidly decomposed using thiosulfate and water. The method provides an inexpensive, safe, and on-site executable way to remove and detoxify methyl bromide from fumigation discharge gases, thereby reducing or eliminating methyl bromide emissions into the atmosphere.

Patent No. 5, 904, 909. Issued: May 18, 1999.

#### MODELING THE FATE AND TRANSPORT OF VOLATILE PESTICIDES

### S.R. Yates, D. Wang, S. Papiernik and J. Gan

Volatilization is a major pathway by which pesticide residues disappear from target areas. This process can be the principal factor affecting efficacy and is a source of unwanted chemicals to the atmosphere. Some volatile pesticides are persistent and can be transported over large distances where they may be deposited in water and soil far removed from their sites of application. Volatile pesticides may also cause other unique problems. For example, methyl bromide, a widely-used soil fumigant, has been shown to damage stratospheric ozone and will soon be phased-out. Since pesticides will likely face increased scrutiny in years ahead, there is a great need to understand the mechanisms that control the emission of pesticides into the atmosphere so that volatilization can be minimized. This paper describes how mathematical models can be used to improve our understanding of pesticide fate and transport and to provide new methods to better manage pesticide application.

American Chemical Society Annual Meeting, New Orleans, Aug. 23, 1999.

#### GEOSTATISTICS AND SPATIAL VARIABILITY OF SOIL PROPERTIES

#### S.R. Yates and A.W. Warrick

It has long been recognized that natural processes are subject to variability in both spatial and temporal domains. For example, Jury et al. (1987) has summarized a large number of studies of the spatial variability of water and transport parameters. They found that the observed coefficient of variation for the saturated hydraulic conductivity can range 50 to 300%, infiltration rate 25 to 100% and parameters describing unsaturated hydraulic conductivity 20 to 350%. Clearly, to address agricultural problems in the presence of spatial variations of this level require powerful tools.

Geostatistical methods are popular tools that have found many uses in the analysis of agricultural problems. The methods are generally used to determine various spatially related quantities that characterize the variability of one or more parameters in space and or time. Simple, ordinary and universal kriging methods produce linear estimators that are useful for obtaining estimates of a spatially distributed property over a region, especially at locations for which no data are available. Work on new geostatistical, methods continues, for example, fuzzy logic has been incorporated into estimation methods (Odeh et al., 1992a,b), more efficient methods for obtaining the cross-variogram have been developed (Clark et al., 1989) and nonparametric and nonlinear methods have been used as a means for obtaining the conditional probability of undesirable events.

In: Skaggs (ed.), Agricultural Drainage, pp.1235-1258, 1999.

### EMISSION OF PESTICIDES INTO THE AIR

### F. van den Berg, G.R. Kubiak, W.G. Benjey, M.S. Majewski, S.R. Yates, G.L. Reeves, H.H. Smelt and A.M.A. van der Linden

During and after the application of a pesticide in agriculture, a substantial fraction of the dosage may enter the atmosphere and be transported over varying distances downwind of the target. The rate and extent of the emission during application, predominantly as spray particle drift, depends primarily on the application method (equipment and technique), the formulation and environmental conditions, whereas the emission after application depends primarily on the properties of the pesticide, soils, crops and environmental conditions. The fraction of the dosage that misses the target area may be high in some cases and more experimental data on this loss term are needed for various application types and weather conditions. Such data are necessary to test spray drift models, and for further model development and verification as well. Following application, the emission of soil fumigants and soil incorporated pesticides into the air can be measured and computed with reasonable accuracy, but further model development is needed to improve the reliability of the model predictions. For soil surface applied pesticides reliable measurement methods are available, but there is not yet a reliable model. Further model development is required which must be verified by field experiments. Few data are available on pesticide volatilization from plants and more field experiments are also needed to study the fate processes on the plants. Once this information is available, a model needs to be developed to predict the volatilization of pesticides from plants, which, again, should be verified with field measurements. For regional emission estimates, a link between data on the temporal and spatial pesticide use and a geographical information system for crops and soils with their characteristics is needed.

Water, Air and Soil Pollution 115:195-218, 1999.

#### REDUCING FUMIGANT EMISSIONS AFTER SOIL APPLICATION

### S.R. Yates, J. Gan, S.K. Papiernik, R. Dungan and D. Wang

Volatilization and soil transformation are major pathways by which pesticides dissipate from treated agricultural soil. Volatilization is a primary source of unwanted agricultural chemicals in the atmosphere and can significantly affect fumigant efficacy. Volatile pesticides may cause other unique problems; for example, the soil fumigant methyl bromide has been shown to damage stratospheric ozone and will soon be phased, out. There is also great concern by persons living near treated fields about the health consequences from inhalation of fumigants. Since replacement fumigants will likely face increased scrutiny in years ahead, there is a great need to understand the mechanisms that control their emission into the atmosphere so these losses can be minimized without loss of efficacy. Recent research has shown that combinations of vapor barriers and soil amendments can be effective in reducing emissions. In this paper, some potential approaches for reducing fumigant emissions to the atmosphere are described.

Phytopathology 90:S103. Publication no. P-2000-0077-SSA, 2000.

### ANALYTICAL SOLUTIONS FOR THE TRANSPORT OF VOLATILE ORGANIC CHEMICALS IN UNSATURATED LAYERED SYSTEMS

### S.R. Yates, S.K. Papiernik, F. Gao and J. Gan

Several analytical solutions were developed that describe the transport of volatile organic chemicals or other gases in layered porous media. Solutions are presented for a one-dimensional system consisting of either two finite soil layers or a finite layer adjacent to an infinite soil layer. The proposed solutions may be useful for studying the movement of volatile chemicals or other gases in layered soils, as well as for gas movement from soils into passive flux chambers, which are commonly used for measuring the surface volatilization rate. The behavior of the solutions is illustrated by several examples showing the soil gas concentration and the flux density as a function of time. At early times it was found that the flux density into a chamber is relatively constant when the mass transfer coefficient *h* is small. However, the concentration at the soil-chamber interface changes rapidly. For large *h*, the flux density at the interface changes rapidly, and the concentration is relatively constant.

Water Resour. Res. 36(8):1993-2000, 2000.

#### PREDICTING PESTICIDE VOLATILIZATION FROM SOILS

### S.R. Yates, S.K. Papiernik, Q.L. Ma and J. Gan

Due to concerns about public health and environmental contamination, there has been great interest in improving our understanding of the processes and mechanisms that affect pesticide emissions from fields. For many situations, predicting pesticide volatilization has been limited to simple situations that often neglect important environmental conditions such as changes in ambient temperature and/or the effect of micrometeorological conditions. Recent research has shown that changes in ambient temperature can strongly affect methyl bromide volatilization under field conditions. Little research has been conducted that couples atmospheric processes to the volatilization of pesticides from soils. A field study was conducted to measure the volatilization of methyl bromide from a 3.5 ha field. Four methods were used to obtain the volatilization rate as a function of time. A one-dimensional numerical model was developed and used to simulate the fate and transport of methyl bromide from the fumigated field. The numerical simulation simultaneously solves water, heat, and solute transport equations including chemical transport in the vapor phase. Three volatilization boundary conditions were used to assess their accuracy in predicting the volatilization rates. The first two boundary conditions follow stagnant boundary layer theory and use no atmospheric information. For these boundary conditions, one assumes isothermal conditions and the other assumes temperature-dependent conditions. The third boundary condition couples soil and atmospheric processes and was found to provide an accurate and credible simulation of the instantaneous volatilization rates compared to a stagnant boundary layer condition. For some information such as cumulative emissions, the simulations for each boundary condition provided similar results. This indicates that simplified methods may be appropriate for obtaining certain information.

4<sup>th</sup> International Conference on Environmetrics and Chemometrics, Las Vegas, NV, Sept. 18-20, 2000.

#### CONTROLLING AGRICULTURAL EMISSIONS OF METHYL BROMIDE

### S.R. Yates, D. Wang, S.K. Papiernik and J. Gan

Over the last 40-50 years methyl bromide (CH3Br) has been used throughout the world to sterilize soils in preparation for planting various high-cash-value fruit and vegetable crops. Highly toxic, CH3Br is very effective in controlling a variety of soil-borne pests, such as nematodes, weeds and fungi. CH3Br has been an important component of agricultural systems in the U.S. and its phase-out is expected to cause financial hardship to agricultural producers. Recent economic assessments estimate that more than \$1.5 billion in annual lost production would occur in the United States alone.

In most commercial operations, CH3Br is applied from a tractor pulling two or more metal shanks that cut into the soil. CH3Br is injected into the soil at approximately 25 cm depth from nozzles on the backside of each shank. Simultaneously, the tractor lays down a 3.5 m wide sheet of 0.025 mm thick high-density polyethylene (HDPE) plastic film; burying one side and gluing the other side to the previous plastic sheet. This creates a series of panels down the field and a continuous cover over the field. Large amounts of CH3Br are applied at rates ranging from 200 to 400 kg/ha.

Emission of CH3Br into the atmosphere is affected to a large degree by the properties of the soil, ambient environmental conditions, application methods, and properties of the plastic film used to seal the surface. Recent research has shown that the traditional HDPE film is largely ineffective in containing CH3Br in soil.

IGACtivities 19:16017, 2000.

### THEORY AND LABORATORY STUDY OF A TALL PASSIVE CHAMBER FOR MEASURING GAS FLUXES AT SOIL SURFACE

#### F. Gao, S.R. Yates, M.A. Anderson and M.V. Yates

A tall passive chamber with a height significantly greater than its horizontal dimensions is proposed for measuring fluxes of volatile organic compounds (VOCs) at soil surface. The significant feature of this tall chamber is the presence of a vertical concentration gradient of the target gas in the chamber due to gas emission from soil. The emission and transport behavior of the target gas in the soil-chamber system are analyzed using diffusion theory. A mathematical model is developed to estimate the flux from the soil into the tall chamber, providing the target gas establishes a detectable vertical concentration gradient in the chamber. To obtain the data required for calculating flux, only two gas concentrations (C1 and C2) at two heights ( $h_1$  and  $h_2$ ) within the chamber need to be measured at the end of a short chamber placement time (Q). To evaluate the applicability of the tall chamber for measuring flux, several laboratory tests have been conducted using methylene chloride and methyl bromide as the target gases. The results indicate that the proposed tall chamber has a promising potential as a laboratory method for measuring fluxes of volatile organic compounds at soil surface.

J. Air & Waste Management Assoc. 51(1):0000, 2000.

### DYNAMISM OF NON-EQUILIBRIUM COMPLEX SYSTEMS AS FLUID FLOW IN SOIL

### R.E. Ernst, S.E. Allaire-Leung and S.R. Yates

Preferential flow (PF) is ubiquitous in soil and many processes contributing to it have been intensively studied. However because of its complexity and dynamism, PF is difficult to predict in field conditions. This presentation introduces a theory developed for such complex dynamic systems. We compare the characteristics of these systems to those of PF. Using information found in the literature, we show that PF has fractal characteristics, some type of chain reaction occurs during wetting and drying processes, temporal fluctuation of PF may follow a power spectrum type of behavior, and water flow tends toward critical states at different spatial and temporal scales. We explore the potential of this theory to combine all types of PF processes for field prediction.

Agronomy Abstract p. 218, 2000.

### 2-D MOVEMENT AND VOLATILIZATION OF FUMIGANTS IN SOILS UNDER DIFFERENT MANAGEMENT METHODS.

### S.E. Allaire-Leung, S.R. Yates and F.F. Ernst

Propargyl bromide (3BP) is an alternative fumigant under consideration to replace methyl bromide for pest control in agricultural production. There is an urgent need to study potential management methods that can reduce atmospheric emission when 3BP is injected in the soil. A 2-D laboratory soil column connected to an automatic gas sampler system was used to compare the movement of 3BP in soil and its volatilization due to different initial soil water contents and irrigation timings. A bed-furrow system was made. A tarp was installed above the bed only, and furrow irrigation was applied at different times after 3BP injection. Volatilization was not always higher in the furrow as compared to the bed. Volatilization decreased with frequent short irrigations compared to a long single irrigation. Higher initial soil water content decreased volatilization. Significant convective gas flux occurred in the column during irrigation leading to less volatilization than models predict. Different time-concentration index distributions were obtained in the profile under different irrigation management methods.

Agronomy Abstract p. 201, 2000.

## Appendix A

### **Technology Transfer Accomplishments for 1999-2000**

### Soil & Water Chemistry Research

### "Salt Sniffer"

We have developed a new commercial grade mobilized salinity assessment unit, designated the "Salt Sniffer." The Unit provides for remote sensing of salinity, with depth profiling information, using two EM-38 units, recently modified by Geonics<sup>TM</sup> (dual-dipole synchronized electromagnetic inductance meter, EM-38DD). As the unit is driven across a field, continuous electrical conductivity data is collected. This conductivity survey data is then instantly merged with spatial location information from a Trimble Pro-XRS real-time GPS receiver, and then stored into the GPS data logger (which can then be conveniently downloaded at the end of the survey process). The assessment platform can also carry a front mounted soil sampling rig (hydraulic push-probe coring equipment). This allows the platform to be used for both signal data acquisition and site-specific soil sampling operations, increasing its versatility and cost-effectiveness. Six additional units are now operational and used by the Bureau of Reclamation for large scale salinity assessment studies in the Lower Colorado Region.

### ESAP-95

The ESAP-95 Software package was developed and released for use with the new mobile salinity assessment equipment. The ESAP-95 software package facilitates the effective use and interpretation of survey conductivity information acquired by nearly all types of mobilized conductivity assessment platforms. (ESAP-95 is an acronym for [E]Ce (salinity) [S]ampling [A]ssessment and [P]rediction software, for Windows 95/98/NT.) This software package was specifically designed to (1) analyze, process, and display automated conductivity survey information, (2) generate optimal soil sampling plans based on the acquired conductivity survey data, (3) convert the survey data into spatial soil salinity information using the soil sample information, and (4) generate field scale salinity inventory statistics, crop yield loss predictions, and spatial salinity maps. The software package employs an easy-to-use, Windows based graphical user interface, and incorporates all of the applied and theoretically based assessment prediction models developed at the Salinity Laboratory since 1989. The software can also be effectively used for multiple types of precision farming sampling applications, in addition to soil salinity inventory and assessment modeling.

### **Lower Colorado Region Salinity Assessment Network**

A cooperative project has been initiated by the George E Brown Jr. Salinity Laboratory and the US Bureau of Reclamation to develop and deploy a salinity assessment network throughout the USBR Lower Colorado Region. This project is being jointly sponsored by the Laboratory's Soil Chemistry and Assessment Research program and the USBR-LCR Water Conservation Field Service program, and coordinated by Chemistry/Assessment personnel. The goal of this project is to foster the growth and development of locally managed salinity assessment programs which can in turn aid

the farmers and growers in each of their service areas. Once deployed, each program will offer rapid soil salinity inventorying and monitoring services, as well as advice on related issues such as soil leaching and reclamation, water conservation, and optimal water management under saline conditions. The five combined, programs are expected to eventually serve more than one million acres of irrigated agriculture throughout the Lower Colorado Region.

This is a three year-applied project with a heavy emphasis on the transfer of currently developed Laboratory assessment technology. The immediate project objectives are (1) to develop and establish five salinity assessment programs throughout the Lower Colorado Region, (2) to assist in the transfer of Laboratory developed hardware and salinity software assessment technology to each assessment team, and (3) to train and instruct the assessment teams at each location in the proper use and implementation of this technology. The five locations selected by the USBR for development of assessment programs are as follows: Coachella Valley, Coachella Valley Resource Conservation District, Imperial Valley, Imperial Irrigation District Yuma Agricultural Center, AZ Parker CA, U.S. Bureau of Indian Affairs, Palo Verde Valley.

### **Boron Adsorption/Transport**

We have developed a relationship to predict the B adsorption parameters of a soil for use in the constant capacitance model. The relationship uses readily available soil properties, thus avoiding the need to conduct time-consuming adsorption studies on each soil. The adsorption characteristics are needed for recommendations regarding reclamation of B affected soils and for development of management systems when irrigating with high B waters. Model will also be useful to nonagricultural users including DOE for predicting B transport and evaluating management options for control in discharge water.

### **Modeling Carbon Dioxide Flux**

We have developed the USGF model for prediction of above canopy carbon dioxide flux. The model combines a version of the UNSATCHEM model predicting water flow, water content and carbon dioxide transport and production in the soil, with the GAS-FLUX model for whole canopy photosynthesis. The model was tested against data obtained at the AmeriFlux Wheat Site in Oklahoma. The model, now available, is suitable for prediction of net ecosystem fluxes, and can be used to evaluate the representation of processes in the large carbon exchange and global circulation models.

### GIS

The GIS-linked solute transport software and salinity assessment technology for preparing maps of salt-affected soils have been demonstrated to the Broadview Water District. David Cone, manager of the Broadview Water District, has received maps inventorying the salt-affected soils for the district as well as maps showing where the greatest salt-loading is occurring within individually farmed fields. This spatial information provides the district with a useful site-specific tool for modifying irrigation and drainage management to reduce salt loads to drainage water and for advising farmers on future crop and irrigation strategies.

### Plant Science & Food Safety Research

An evaluation of salt and boron tolerance of eucalyptus trees for the University of California/Salinity Drainage Program, Prosser Trust, and California Department of Water Resources was completed. Crop and water use functions were developed for the management of eucalyptus trees grown in agroforestry plantations and irrigated with brackish waters in the San Joaquin Valley (SJV). In response to irrigation with boron-contaminated saline waters, the trees grew poorly, were inefficient water users, and did not meet the requirements necessary for drainage water reuse programs. As a result, research priorities of state and federal agencies have been redirected to alternative cropping and management systems.

A two-year study has been initiated for the University of California/Salinity Drainage Program to identify useful crops for production potential in sequential water reuse systems. High quality forage crops are currently in short supply in the Central Valley. Therefore, forage species, including alfalfa, trefoils, paspalum, alkali sacaton, tall wheatgrass, kikuyu grass, and bermuda, are under evaluation at moderate (15 dS/m) and high (25 dS/m) salinities. The interactive effects of salinity and potentially toxic trace elements (Se and Mo) on forage yield and nutritive quality will be determined. The information developed will benefit growers in the SJV in two ways: by providing management options that will reduce the volumes of saline drainage effluents and at the same time, by offering the opportunity to fill the unmet needs for high quality forages.

A study of host-insect pest interactions is in its third, and final year, for the University of California/Salinity Drainage Program. To date, 62 *Atriplex* accessions have been screened for high salt tolerance and their ability to accumulate Se from saline substrates of different ion composition (e. g. chloride- or sulfate-dominated). The effect of leaf-Se on survival, development, and behavior of the lepidopteran pest, *Spodoptera exigua*, and the insect vector of curly top diseases, *Circulifer tenellus* (beet leafhopper) is under investigation. Information on Se biomagnification e. g. from insect to avians and fish, will be determined.

Lesquerella (Lesquerella fendleri) produces a seed oil that has desirable industrial applications. A.genotype, WCL-SL1, with improved salt tolerance was developed in cooperation with the ARS-USDA Water Conservation Laboratory, Phoenix, AZ. The new lesquerella selection was registered with the Crop Science Society and seed was deposited in the National Seed Storage Laboratory. Several growers and plant breeders have obtained seed with the intentions of testing the crop at selected sites in Arizona and New Mexico.

Provided advice to numerous national and international students, home owners, growers, consultants, farm advisors, extension specialists, and university scientists on salinity-fertility interactions and many aspects of salt and boron tolerance of various plant species.

### Soil Physics & Pesticide Research

#### **Pesticide Detoxification**

We have developed a simple, safe and cost-effective method to reclaim activated carbon that has been contaminated with methyl bromide or other similar fumigation gases (e.g. methyl iodide, chloropicrin, 1,3-dichloropropene, propargyl bromide). The process uses activated charcoal that has been wetted with a thiosulfate-containing solution to trap and destroy the fumigation gas. The chemical reaction produces harmless by-products. The method only requires that fumigation gases be pumped through a charcoal bed containing a thiosulfate solution and this could be easily accomplished at the fumigation site. The only disadvantage of this method is that the fumigation gase is not recovered for reuse. However, this is of minor consequence since most fumigation gases are relatively inexpensive. A related patent was developed to quickly and inexpensively destroy certain fumigants used in containment structures, eliminating emissions to the atmosphere.

This research has been further extended by the discovery that thiosulfate salts will also degrade another class of pesticides, the chloroacetamides, which includes alachlor, metalochlor, propachlor and acetochlor. Adding thiosulfate salts to contaminated (i.e., from spillage) or treated soil provides a means for detoxifying pesticide residues in soil.

### **New Method To Determine the Permeability of Agricultural Films**

Plastic tarps are currently used during soil fumigation to control fumigant emissions to the atmosphere. These films have been shown to be permeable to fumigant vapors and result in appreciable losses to the atmosphere. New low-permeability films are being developed to reduce fumigant emissions and increase efficacy. A rapid, reliable and sensitive method has been developed to measure the permeability of agricultural films to fumigant vapors, an integral part of any new management practice. To create a standardized method, the method estimates the mass transfer coefficient of fumigant compounds across agricultural films. The mass transfer coefficient is a measure of the film's resistance to chemical diffusion. The mass transfer coefficient is a fundamental property of the film-chemical combination and independent of the concentration gradient across the film. This method uses static sealed cells; fumigant vapor is spiked to one side of the film and the concentrations on both sides of the film are monitored until equilibrium. A mathematical model is fitted to the data to obtain the mass transfer coefficient. The method will be submitted to ASTM for possible adoption as a standard method.

### **Computer Software**

The Soil Physics group over the years developed a large number of computer models to predict the movement of water and dissolved chemicals (pesticides, fertilizers, salts, toxic trace metals) in soils and groundwater. Since 1990 some 6000 copies have been made available upon request to a variety of users worldwide (universities, soil and groundwater professionals, private consulting firms, extension personnel, and users in a such federal agencies such as NRCS, DOE, EPA, NRC, USGS, NASA and NOAA). Additionally, copies are being distributed by EPA, the International Ground

Water Modeling Center (IGWMC) of the Colorado School of Mines (Golden, CO), and several software clearing houses; several codes can be downloaded directly from USSL's web site (www.ussl.ars.usda.gov/MODELS/MODELS.HTM).

Two of the models (the windows-based HYDRUS-1D and -2D software packages) are being used to predict water, solute and/or heat movement in the unsaturated zone between the soil surface and the groundwater table, including groundwater itself. The models are being distributed through a CRADA between IGWMC and ARS. The software packages are being used not only for typical agricultural applications (such as for irrigation and drainage management, virus and pesticide transport, and soil salinization or reclamation studies), but also many for soil and ground water pollution (and remediation) studies involving non-agricultural chemicals (such as radioactive waste, as well as pollutants being released from industrial and municipal waste disposal sites). The CRADA has been extremely beneficial to both ARS and IGWMC by facilitating a more effective distribution of the software to a variety of users in research and management, reaching users outside of traditional agriculture, providing faster service to customers, providing interaction among users through a web-based electronic user group, and obtaining critical feedback on how to further improve the software.

### **Hydraulic Characterization of the Vadose Zone**

Computer models are now increasingly used in research and management to study or predict water flow and solute transport processes in the unsaturated (vadose) zone between the soil surface and the groundwater table. The unsaturated hydraulic functions are key input data for such models. These functions can be either measured directly at great cost, or estimated more conveniently in an indirect manner from more easily measured data based using pedotransfer functions. During the past year we released a powerful windows-based program (Rosetta, version 1.0) to rapidly estimate the unsaturated hydraulic properties from surrogate soil data such as soil texture and bulk density.

Rosetta uses neural network analysis to estimate the soil water retention and unsaturated hydraulic conductivity functions, and their uncertainty, in a hierarchical manner from limited data (such as soil textural class) to more extensive input data sets (such as sand, silt and clay percentages and the bulk density). This hierarchical approach is of a great practical value because it permits optimal use of available input data. The program is finding widespread application in subsurface flow and transport problems, and in studies of regional and global climate. NASA, DOE, NRCS, USGS and EPA are among its users. Rosetta can be downloaded directly from the USSL's web site: www.ussl.ars.usda.gov/MODELS/rosetta/rosetta.htm.